Monday, March 5, 2007 8:00AM - 11:00AM – Session A4 DPOLY DMP GSNP: Responsive and Adaptable Polymeric Materials  Colorado Convention Center Korbel 2B-3B

8:00AM A4.00001 Adaptive and Responsive Polymer NanoComposites RICHARD VAIA, Air Force Research Laboratory — In addition to thermal-mechanical improvements of commodity plastics, polymer nanocomposite concepts offer opportunities to impart responsive characteristics as well as enhance the performance of active polymers, including shape memory and piezo-resistivity. Opportunities arise from: 1) the utilization of the extensive polymer-nanoparticle interfacial area (>500 m²/g), 2) the responsiveness of the percolative network of the nanoparticle to external fields, and 3) the impact of nanoscale compositional fluctuations on the local electric field. As an example, carbon nanotube addition to shape memory polymers increases blocking stress by 100% and provides novel electrical and optical methods to trigger recovery. Similarly, the pyro-resitive character of carbon nanotube – polimide nanocomposites depends on the surface modification of the nanotube, displaying a positive coefficient of resistivity (resistance increase with temperature) from cryogenic to the glass transition temperature. Challenges facing characterization and the establishment of structure-property correlations will be discussed.

8:36AM A4.00002 Hydrophobic Hydration of Stimulus-Responsive Polyproteins Measured by Single Molecule Force Spectroscopy*, STEFAN ZAUSCHER, Duke University — We present a new procedure to reduce and analyze force-extension data obtained by single molecule force spectroscopy (SMFS). This approach allows, for the first time, to infer effects of solvent quality and minor changes in molecular architecture on molecular-elasticity of individual (bio)macromolecules. Specifically, we show how changes in the effective Kuhn segment length can be used to interpret the hydrophobic hydration behavior of elastin-like polypeptides (ELPs). Our results are intriguing as they suggest that SMFS in combination with our analysis procedure can be used to study the subtleties of polypeptide-water interactions on the single molecule level. We also report on force-induced cis-trans isomerization of prolines, which are repeated every fifth residue in the main chain of ELPs. We present evidence for this mechanism by Monte Carlo simulations of the force-extension curves using an elastically coupled two-state system. Our results suggest that SMFS could be used to assay proline cis-trans isomerization in proteins and may thus have significant potential diagnostic utility.

9:12AM A4.00003 Nature’s Mechanisms for Tough, Self-healing Polymers and Polymer Adhesives, PAUL HANSMA, University of California — Spider silk and the natural polymer adhesives in abalone shells and bone can give us insights into nature’s mechanisms for tough, self-healing polymers and polymer adhesives. The natural polymer adhesives in biomaterials have been optimized by evolution. An optimized polymer adhesive has five characteristics. 1) It holds together the strong elements of the composite. 2) It yields just before the strong elements would otherwise break. 3) It dissipates large amounts of energy as it yields. 4) It self-heals after it yields. 5) It takes just a few percent by weight. Both natural polymer adhesives and silk rely on sacrificial bonds and hidden length for toughness and self-healing. A relatively large energy, of order 100 eV, is required to stretch a polymer molecule after a weak bond, a sacrificial bond, breaks and liberates hidden length, which was previously hidden, typically in a loop or folded domain, from whatever was stretching the polymer. The bond is called sacrificial if it breaks at forces well below the forces that could otherwise break the polymer backbone, typically greater than 1nN. In many biological cases, the breaking of sacrificial bonds has been found to be reversible, thereby also providing a ‘self-healing’ property to the material. Individual polymer adhesive molecules based on sacrificial bonds and hidden length can supply forces of order 300pN over distances of 100s of nanometers. Model calculations show that a few percent weight of sacrificial bonds and hidden length can give high performance composite materials including nanotube and graphene sheet composites.

9:48AM A4.00004 Cell microrheology in health and disease” be suitable for your session, DENIS WIRTZ, Johns Hopkins University — No abstract available.

10:24AM A4.00005 Is experimental heteropolymer sequence design practical, or does it belong to the realm of science fiction?, ALEXANDER GROSBERG, Physics Department University of Minnesota — In the protein folding context, theorists consider various methods of sequence design, which turns out a very useful way to look at various heteropolymer properties. Simultaneously and largely independently, there is a rather old idea to find an experimental counterpart of computational and theoretical sequence design algorithms. Here, we review some of the experiments in this direction along with some of the more recent theoretical advances and come to the guarded conclusion that full experimental realization of sequence design is possible but probably remote.

Monday, March 5, 2007 8:00AM - 10:24AM – Session A8 DMP: Focus Session: Novel Superconductors I: Doping and Impurities in MgB2 Colorado Convention Center Korbel 1C

8:00AM A8.00001 MgB2: doped or with pressure, four systems same behaviour, PABLO DE LA MORA, SABINA RUIZ-CHAVARRIA, ULISES ESTEVEZ, Fac. de Ciencias, GUSTAVO TAVIZON, Fac. de Quimica, UNAM, Mexico, D.F. — MgB2, the intermediate Tc superconductor, can be doped with carbon, aluminium and scandium and it has been also studied experimentally under pressure, in these four cases Tc diminishes. In previous studies we have shown, with electronic structure calculations, that when Mg is substituted with Sc ([Mg,Sc]B2) the drop of Tc can be associated with the loss of electrical anisotropy of the σ-bands [1]. When Mg is substituted with Al ([Mg,Al]B2) or B is substituted with C ([Mg,B,C]2) then, with a change of doping scale, a common Tc curve is obtained for both systems, comparison with the σ-DOS shows that Tc drop is due to σ-band-filling and to σ-band anisotropy loss [2]. In further studies we have found that both these features, σ-band anisotropy reduction and the loss of σ-band-carriers, can be associated to the drop of Tc, in these three doped systems [Mg(B,C)2], Mg,Al]B2 and [Mg,Sc]B2 and in MgB2 under pressure. All these studies show that (a) with a change of doping scale then Tc in both the C and Al doped systems follows the same curve which is very close to the σ-DOS, (b) for the four systems both the σ-band anisotropy and the number of σ-carriers are two fundamental physical properties of the relatively high Tc in MgB2. [1] J. Phys.: Condens. Matter 18 (2006) 1403-1412 [2] cond-mat/060619
8:12AM A8.00022 First principles study of the electronic structure and phonon properties for Al and C-doped MgB$_2$. O. DE LA PEÑA-SEAMAN, R. DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico; R. HEID, K.-P. BOHNEN, Institut fuer Festkoerperphysik, Forschungszentrum Karlsruhe, Germany. — We have studied the structural, electronic and lattice dynamic properties of the superconducting alloys Al and C-doped MgB$_2$ within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. For both systems the structural parameters were determined on the following ranges, $0<x<1$ for Mg$_{1-x}$Al$_x$B$_2$ and $0<x<0.4$ for MgB$_2$C$_x$, finding a very good agreement between the calculated structural parameters and experimental data. The complete phonon dispersion curves were selected for selected Al and C-concentrations. The calculated phonon bands for MgB$_2$ using the LDA and GGA approximations are compared in detail with the experimental data available in the literature. The evolution of the full-dispersion curves are analyzed as a function of Al and C-concentration, specially the E$_{2g}$-phonon mode frequency. In agreement with the experimental observed behavior, we find strong renormalization of the E$_{2g}$-mode for both Al and C-doped MgB$_2$. Additionally, we found a strong reduction of the E$_{2g}$-band dispersion with the filling of the $\sigma$-band. This research was supported by CONACYT, Mexico under Grant No. 43830-F.

8:24AM A8.00033 Carbon and Aluminum Doping in MgB$_2$. Similarities and differences, PETER SAMUELY, PAVOL SZABO, ZUZANA HOLANOVA, Centre of Low Temperature Physics IEP Slovak Academy of Sciences, SK-04001 Kosice, Slovakia, MANUEL ANGST, RUDGERE WILKE, SERGEY BUD'KO, PAUL CANFIELD, Ames Laboratory and Iowa State University, Ames, IA 50011, USA. — Both carbon and aluminum dope the magnesium diboride by one extra electron which leads to filling of the most important $\sigma$ band and decreasing of the transition temperature. The point-contact spectroscopy in magnetic field is used to address the evolution of two superconducting energy gaps and density of states in the doped systems with $T_c$ from 39 to 22 K. The similarities and differences in the inferred interband and intraband scatterings introduced by these two substitutions are discussed. It is shown that the gap superconductivity is retained in all studied cases. The carbon doping is effective in increasing of the intraband scattering mainly in the $\pi$ band. This leads to important enhancement of the upper critical field. The approaching of two gaps is stronger in the Al-doped systems but the interband scattering is not very sensitive on the carbon doping, in the samples with $T_c$'s below 10 – 15 K. Al substitution does not affect strongly the intraband scattering leaving the samples in the clean limit.

8:36AM A8.00034 Carbon Doped MgB2 Thin Films using TMB. R.H.T. WILKE, QI LI, Department of Physics, Pennsylvania State University, X.X. XI, Department of Physics, Department of Materials Science and Engineering, Pennsylvania State University, D.R. LAMBORN, Department of Chemical Engineering, Pennsylvania State University, J. REDWING, Department of Materials Science, Pennsylvania State University. — The most effective method to enhance the upper critical field in MgB$_2$ is through carbon doping. In the case of thin films, “allying” with carbon has resulted in enhanced H$_c$ values estimated to be as high as 70 T for H parallel to ab and 40 T for H perpendicular to ab [1]. “Alloying” refers to the in-situ Hybrid Physical-Chemical Vapor Deposition (HCPVD) of carbon containing MgB$_2$ films using (CSH)52Mg as the carbon source. While these films exhibit enhanced Hc2 values, there are amorphous boron- carbon phases in the grain boundaries that reduce the cross section area for superconducting current. We present here the results of our attempts to make more homogeneously carbon doped thin films using gaseous trimethyl-boron (TMB) as the carbon source. Initial results indicate different behavior upon carbon doping using TMB from carbon-alloying. The microstructures and upper critical fields of the carbon doped films using TMB and carbon alloyed films will be compared. [1] V. Braccini et al., Phys. Rev. B 71 (2005) 012504. [2] A.V. Pogrebnyakov et al., Appl. Phys.lett 85 (2004) 2017.

8:48AM A8.00035 Disorder in carbon-doped-HPCVD MgB$_2$ thin films. YE ZHU, P.M. VOYLES, Department of Materials Science and Engineering, University of Wisconsin, Madison, A.V. POGREBNYAKOV, X.X. XI, Department of Physics, University of Wisconsin, Madison, X. XU, Department of Materials Science and Engineering, University of Wisconsin, Madison. — The structural, electronic and lattice dynamic properties of MgB$_2$ films prepared by hybrid physical-chemical vapor deposition have the highest $H_{c2}$ (~70 T at 0 K for H parallel to ab plane) of all MgB$_2$ materials. We have characterized the nanoscale structure and chemistry of one such film by TEM and STEM. The C concentration in the MgB$_{1-x}$C$_x$ grains from EELS is not dramatically higher than that of C-doped bulk MgB$_2$, so doping does not explain the high $H_{c2}$. Instead, the doped film has a variety of forms of structural disorder at length scales down to 5 nm, which may be sufficient to explain the $H_{c2}$ of these films. These include MgB$_2$ domains with a 30 degree rotation about the a-axis, small angle rotations about c-axis, and a small tilt of the c-axis. There are also amorphous, C-rich regions between some MgB$_2$ domains. The amorphous phase comes from the oversupply of C during growth, which may also cause the other disorder by interrupting epitaxial film growth. This work is supported by the FRG on MgB$_2$, NSF DMR-0514592.

9:00AM A8.00036 Correlated enhancement of $H_c$ and J in carbon nanotube-doped MgB$_2$. M. JAIME, MPA-NHMFL, LANL, Los Alamos, NM 87544, A. SERQUIS, G. SERRANO, S. MORENO, CAB, Bariloche, Argentina, L. CIVALE, B. MAIOROV, M. JAIME, MPA-NHMFL, LANL, Los Alamos, NM 87544, F. BALAKIREV, MPA-NHMFL, LANL, Los Alamos, NM 87544 — We achieved simultaneous enhancement of upper critical magnetic field, $H_{c2}$, and critical current density, $J_c$, by doping polycrystalline samples of MgB$_2$ with double-wall carbon nanotubes (DWCNT), a source of atomic carbon. The optimum DWNT content from the point of view of the $J_c$ is in the range 2.5-10% at depending on field and temperature. Record values for $H_{c2}$($T_c$) are obtained in the samples with $H_{c2}$($T_c$) = 46 T at 20 K. 21 T) are obtained in the carbon nanotube-doped MgB$_2$ thin samples with 10% at DWNT content. The measured $H_{c2}$ vs T in all samples is successfully described using a theoretical model for a two-gap superconductor in the dirty limit first proposed by Gurevich et al.

9:12AM A8.00037 Point-Contact Andreev-Reflection Spectroscopy in Neutron-Irradiated MgB$_2$. R.S. GONNELLI, A. CALZOLARI, D. DAGHERO, M. TORTELLO, G.A. UMMARINO, Dipartimento di Fisica and CNISM, Politecnico di Torino, Italy; V. A. CREPPE, P.N. Lebedev Physical Institute, RAS, Moscow, Russia; C. TARANTINI, Cnr-INFN-LAMIA and Dip.to di Chimica e Chimica Industriale, Universita di Genova, Italy. — We report recent results of point-contact spectroscopy (PCS) in MgB$_2$ polycrystalline samples irradiated with neutrons at different fluences up to $\Phi = 1.4 \times 10^{20}$ cm$^{-2}$. A strong depression of the bulk critical temperature $T_c$ down to about 8 K was observed after irradiation. The gaps $\Delta_x$ and $\Delta_y$ were obtained from the experimental Andreev-reflection conductance curves through a two-band Blonder-Tinkham-Klapwijk fit and reported as a function of the Andreev critical temperature of the junctions, $T_A$. The resulting $\Delta_x(T_A)$ and $\Delta_y(T_A)$ curves clearly show a merging of the gaps when $T_A < 5$ K, which perfectly confirms the findings of recent specific-heat measurements in the same sample. “Anomalous” contacts with $T_A^c > T_c$ and a different dependence of the gaps on $T_A$ with respect to “standard” ones were obtained in samples irradiated at the highest fluences. The possible origin of these anomalies is discussed in terms of local current-induced annealing and/or nanoscale inhomogeneities - indeed observed by STM in the most irradiated samples.

9:24AM A8.00038 Reflection of two band transitions in the magnetic penetration depth of ion irradiated MgB$_2$. S.D. KAUSHIK, S. PATNAIK, School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110067 — Multiband superconductivity in MgB$_2$ has wide ranging ramifications for its transport characteristics. Using ion irradiation we have previously reported that by carefully choosing the type and density of defects, it is possible to control the intra and inter band scattering between the 2D $\sigma$ and isotropic $\pi$ bands of MgB$_2$. Here we report on the reflection of this defect induced modified scattering mechanism on the Meissner and mixed state penetration depth as a function of temperature, dc magnetic field, and defect density. The measurements are carried out using an ultrastable rf tunnel diode oscillator. The samples include unirradiated and those irradiated with 200 MeV Au$^{117+}$ and 100 MeV Si$^{28+}$. The fits to the superfluid density over the entire temperature range give information about the evolution of two gaps with progressive defecting. From the mixed state measurements the bulk pinning force constant and flux flow resistivity are estimated. We also superconduct the superconducting properties of MgB$_2$ with 2H-NbSe$_2$ ($T_c = 7.3$ K). This work was funded by DST & CSIR, India.
9:36AM A8.00009 Disorder induced evolution of two energy gaps in MgB$_2$\footnote{This work is based on work supported by the National Science Foundation under grant No. 0351449.}. YONG-JIHN KIM. University of Puerto Rico — We study disorder effect on MgB$_2$ superconductivity using the two band model by Suhl, Matthias, and Walker. We stress the importance of the Cooper pair size effect in the response of the BCS superconductor to the perturbation: the bounded Cooper pairs see the impurities within the range of the coherence length. This effect will undermine the initial decrease of the Tc and the big energy gap due to disorder, until the resistance ratio reaches about $\sim 3$. For the resistance ratio less than 3, weak localization starts to decouple electrons and phonons, leading to the significant decrease of both the Tc and the big gap in particular, we trace the evolution of two energy gaps of MgB$_2$ as a function of disorder. Estimating the inter-band scattering rate from the experimental data, we compare our calculations with experiments. We also calculate the transition temperature, Tc as a function of the resistance ratio.

9:48AM A8.00010 Effects of Magnetic and Non-Magnetic Impurities in MgB$_2$: A Point-Contact Study of Single Crystals\footnote{The work was supported by the USDOE(DE-FG02-03ER46064) at BSC and DOUGLAS BONN, University of British Columbia — No abstract available.}. D. DAGHERO. Dipartimento di Fisica e CNISM, Politecnico di Torino, Italy — We studied the effects of chemical substitutions, either magnetic (Mn) or non-magnetic (Al, C), on the energy gaps of MgB$_2$ by means of directional point-contact spectroscopy (PCS) in state-of-the-art single crystals. Here we discuss two noticeable cases, i.e. Mg$_{1-x}$Mn$_x$B$_2$ crystals with $x$ up to 0.015, and Mg$_{1-x}$Al$_x$B$_2$ crystals with $x$ up to 0.32. In both cases, we used a pressure-less PCS technique in which a thin Au wire is put in contact with the side surface of the crystal by means of a small drop of Ag paint. The gaps $\Delta_T$ and $\Delta_T$ were obtained through a two-band Blonder-Tinkham-Klapwijk (BTK) fit of the Andreev-reflection conductance curves of the resulting contacts. Both in Mn- and Al-doped MgB$_2$, the gaps decrease on decreasing the critical temperature of the contacts, $T_c^\text{\lambda}$ (at which the Andreev-reflection structures disappear), but remain clearly distinct down to $T_c^\text{\lambda} \approx 10$ K. Once analysed within the two-band Eliashberg theory, the $\Delta_T$ and $\Delta_T$ vs. $T_c^\text{\lambda}$ curves give information about the effects of Mn and Al substitutions on the different scattering channels (interband and intraband, magnetic or non-magnetic). It turns out that the main effect of Mn is to increase the spin-flip scattering within the $\sigma$ band (with smaller contributions from either the $\pi - \pi$ or the $\sigma - \pi$ channels), as also confirmed by first-principle bandstructure calculations. In the case of Al, the band-filling effect is largely dominant. An increase in non-magnetic interband scattering is possible, but small enough not to give rise to gap merging. In collaboration with G.A. Ummarino, A. Calzolari, M. Tortello, D. Delaude, R.S. Gonnelli, Dipartimento di Fisica and CNISM, Politecnico di Torino, Italy; V.A. Stepanov, P.N. Lebedev Physical Institute, RAS, Moscow, Russia; N.D. Zhigadlo, J. Karpinski, Laboratory for Solid State Physics, ETHZ, Zurich, Switzerland; and S. Massidda, Dipartimento di Fisica, Università di Cagliari, Italy.

Monday, March 5, 2007 8:00AM - 11:00AM — Session A9 DMP: Superconductivity: Thermodynamic and Doping Effects Colorado Convention Center

8:00AM A9.00001 YBCO at the border between antiferromagnetism and superconductivity\footnote{We gratefully acknowledge the support of NSERC and the CIAR.}. DOUGLAS BONN, University of British Columbia — No abstract available.

8:36AM A9.00002 Investigation of the Mössbauer spectrum of RuSr$_2$GdCu$_2$O$_8$ as a function of Temperature shows that there is only one type Ru site\footnote{The work was supported by the USDOE(92-03ER46064) at BSC}. COFFEE, Dept. of Physics, Buffalo State College, NY14222, HARMON, B. GRAVES, N. MILLER, M. DEMARCO, Dept. of Physics, Buffalo State College, NY 14222, DABBROWSKI, S. KOLESNIK, M. MAXWELL. Dept. of Physics, Northern Illinois University, IL 60015, TOORONGIAN, M. HAKA, Nuclear Medicine Department, SUNY Buffalo, NY 14260 — A sample of RuSr$_2$GdCu$_2$O$_8$ was prepared with enriched $^{99}$Ru which allows us to study the temperature dependence of the Mössbauer spectrum up 145K. The sample magnetically orders at 138K and has a transition to superconductivity at 8.7K with an onset at 2A sample magnetically orders at 138K and has a transition to superconductivity at 8.7K with an onset at $\sim 3$. The hyperfine field is 59.4K with isomer shift which indicates that the charge state of the Ru ion is close to +5. The strength of the electric quadrupole interaction is $0.36$ mm/sec with $\eta = 0.2$. This spectrum is essentially identical to that found for a sample prepared with the natural $^{99}$Ru abundance. At 146K, above the magnetic transition temperature, the spectrum is fit with a pure electric quadrupole interaction of the same magnitude as at 4.2K with the same isomer shift.

8:48AM A9.00003 Magnetic Penetration Depth in Overdoped Tl-2201 Superconductors\footnote{We gratefully acknowledge the support of NSERC and the CIAR.}. JESS H. BREWER, SCOTT STUBBS, DARREN PEETS, RUIXING LIANG, WALTER HARDY, DOUG BONN, Univ. of British Columbia, PETER RUSSO, TRIUMF, JEFF SONIER, Simon Fraser Univ. — Studies of the magnetic penetration depth $\lambda_{ab}$, via the $\mu^+$SR lineshape in the vortex state has revealed a great deal about underdoped cuprate superconductors, including the original confirmation of $d$-wave superconductivity. However, overdoped cuprates have been neglected, partly due to the difficulty of doping sufficiently to decrease $T_c$, and partly because the overdoped materials are thought to be “ordinary Fermi liquid” superconductors, about which many presume we already know everything. In the belief that we may not know everything about these materials, the UB group has set out to grow high quality crystals of Tl$_2$Ba$_2$CuO$_{6+x}$ (TI-2201), which can be made very overdoped, to the point of $T_c \rightarrow 0$. We have now used $\mu^+$SR lineshape studies to measure $\lambda_{ab}$ as a function of $T$ and $H$ for crystal mosaics with $T_c$'s of 72, 60 and 46 K. As expected, $\lambda_{ab}^2(T = 0)$ continues to increase with doping beyond optimal doping, but then decreases again with higher doping. We also find a strong dependence on the applied field $H$. The low-$T$ behavior of $\lambda_{ab}^2(T)$ is again strongly linear, as expected for a $d$-wave superconductor.

9:00AM A9.00004 Nodeless $d$-wave superconducting pairing in antiferromagnetic underdoped Pr$_{2-x}$Ce$_x$CuO$_{4-d}$. TAMNOY DAS, R.S. MARKIEWICZ, A. BANSIL, Northeastern University — Experimental results concerning the superconducting pairing symmetry have been contradictory in electron doped cuprates. In particular, penetration depth measurements appear to indicate the presence of an $s$-wave and/or a $d$-wave gap in different doping regimes \cite{1}. Here, we discuss the doping and $T$-dependence of the penetration depth in Pr$_{2-x}$Ce$_x$CuO$_{4-d}$ (PCCO) and provide a natural explanation for the occurrence of a nodeless superconducting gap and a nonmonotonic gap variation with maximum gap near hot-spots in the underdoped system \cite{2}. Despite the presence of a $d_{x^2-y^2}$ pairing gap, we find a crossover of the low-$T$ penetration depth from a nodeless behavior in the underdoped case to a linear-in-$T$ behavior (characteristic of $d$-wave) as doping increases and a nodal Fermi surface pocket emerges. The present results support the coexistence of antiferromagnetism and superconductivity in the electron doped cuprates \cite{3}. Work supported in part by the USDOE.

\begin{itemize}
\end{itemize}
9:12AM A9.00005 Small $T_{c1}^{-1}$ peak near $T_c$ in unconventional BCS superconductors, DAVID PARKER, MPIPKS, STEPHAN HAAS, USC Dept. of Physics and Astronomy — It is usually believed that a coherence peak just below $T_c$ in the nuclear spin lattice relaxation rate $T_{c1}^{-1}$ in superconducting materials is a signature of conventional s-wave pairing. We demonstrate that any unconventional superconductor obeying BCS pure-case weak-coupling theory should show a small $T_{c1}^{-1}$ coherence peak near $T_c$, generally with a height between 3 and 15 percent greater than the value at $T_c$. It is due to impurity scattering, magnetic effects, gap anisotropy and other effects that this peak has not been commonly observed.

9:24AM A9.00006 A Practical Algorithm for Fitting Magnetic Moment Data for Superconducting Thin Films and Multilayers in Parallel Magnetic Fields, SERGII KRYUKOV, WENTAO XU, LANCE DE LONG, University of Kentucky — Superconducting thin films and multilayers in DC magnetic fields applied nearly parallel to the film plane can yield spurious magnetization data dominated by extreme shape anisotropy and strong diamagnetism of a confined supercurrent. This situation may lead to highly reproducible discontinuities or apparently random “instabilities” when measured with SQUID magnetometers such as the ubiquitous Quantum Design MPMS, which requires samples to behave as an ideal point-dipole. We have devised an accurate multipole fitting routine for the raw SQUID voltmeter output that eliminates spurious contributions to the axial dipole moment from transverse (off-axis dipole) or non-point-dipole axial magnetizations. We demonstrate this method as applied to Nb/Ni multilayers and Nb thin films and foils of various thicknesses that probe the influence of supercurrent confinement on the non-dipole response.

9:36AM A9.00007 Magnetic Instabilities along the Superconducting Phase Boundary of Nb/Ni Multilayers, WENTAO XU, AMISH JOSHI, SERGII KRYUKOV, LANCE DE LONG, University of Kentucky, ELYVIRA GONZALEZ, ELENA NAVARRO, JAVIER VILLEGAS, JOSE VICENT, Universidad Complutense Madrid — We report vibrating reed and SQUID magnetometer data that exhibit prominent cusps or oscillations of the SC onset temperature. $\Delta T_{c}(H) \approx 0.01$ to 0.7 K, for a [Nb(23nm)/Ni(5nm)]$_5$ multilayer (ML) in DC magnetic fields applied nearly parallel to the ML plane. The vibrating reed data exhibit additional structures below $T_c$ that may mark multiple SC transitions or vortex-lattice rearrangements within the ML. This striking behavior would then pose new challenges for theoretical and experimental investigations of SC/FCM interfaces that involve “pH phase shifts” of the SC order parameter and exotic (“LOFF”) pairing states. Alternatively, the anomalies may signal dynamical instabilities within a confined, strongly anisotropic Abrikosov vortex lattice.

9:48AM A9.00008 X-ray Structural Studies of HgBa$_2$Cu$_{O+\delta}$O$_{4-\delta}$, C. CHABOT-COUTURE, Stanford U., J. N. HANCOCK, SSRL, L. LU, Stanford U., A. BIANCONI, Università di Roma, F. BRIDGES, UC Santa Cruz, Z. ISLAM, APS, ANL, H. OYANAGI, AIST, Y.-C. CHO, SSRL, Y. LI, G. YU, Stanford U., X. ZHAO, SSRL, M. GREVEN, Stanford University — In recent years, there has been mounting evidence for electronic and structural inhomogeneities in the cuprate high-temperature superconductors (HTSC). From stripe phases found in lanthanum-based cuprates to the oxygen-order-driven lattice modulations in YBa$_2$Cu$_3$O$_{7-\delta}$ and to the nanoscale electronic density-of-states “patches” in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ and other cuprates, these inhomogeneities appear to have significant effects on the electronic, transport, and spectroscopic properties of these systems. Of all the high-$T_c$ materials, HgBa$_2$Cu$_{O+\delta}$O$_{4-\delta}$ has the highest transition temperature among single-layer compounds and one of the simplest structures. Consequently, it may be the perfect candidate system to help separate the effects of extrinsic structural inhomogeneities from those that are universal and intrinsic to HTSC. To begin to address this issue, we have grown sizable, high-quality crystals of HgBa$_2$Cu$_{O+\delta}$O$_{4-\delta}$ and carried out two structural studies: a diffuse x-ray scattering experiment, showing evidence for short-range structural displacement modulations, and a polarized extended x-ray absorption fine-structure (EXAFS) experiment on the temperature-dependent local structure around the copper and mercury atoms.

10:00AM A9.00009 Microscopic origin of the oxygen reduction process and its impact on superconductivity in electron-doped copper oxides, HYE JUNG KANG, University of Tennessee, NIST, University of Maryland, PENCHEENG DAI, University of Tennessee, ORNL, BRANTON J. CAMPBELL, Brigham Young University, PETER J. CHUPAS, STEPHAN ROSENKRANZ, PETER L. LEE, Argonne National Laboratory, QINGZHEN HUANG, NIST, SHILIANG LI, University of Tennessee, SEIKI KOMIYA, YOICHI ANDO, CRIEPI, Japan — The oxygen reduction process is one of the unique processes in the electron-doped high temperature copper oxides. Superconductivity is induced when the electron-doped as grown samples are annealed in the oxygen reduced atmosphere. Many experiments show that a small amount of oxygen reduction affects the nodal gap slope. The implications of our results on the mechanism of cuprate superconductors are discussed based on the Fermi arc picture of normal state. The YBCO single crystal was provided by Prof. Xin Yao at Shanghai Jiaotong University, China.

10:12AM A9.00010 X-ray diffuse scattering experiments from bismuth based high $T_c$ superconductors, M. IZQUIERDO, 1, S. MEGTERT, 2, P. A. ALBOUY, 3, J. AVILA, 1, M. A. VALBUENA, 2, G. GU, 4, J. S. ABELL, G. YANG, 5, M.C. KRYUKOV, 1, R. COMES, 2 (1) University of Bordeaux, UBO, UPR 8554, (2) University of Strasbourg, UHP, CNRS UMR 7198, France — A detailed x-ray diffuse scattering study of the recently found two dimensional (2D) displacive short range order (SRO) superstructure, with doubled periodicity along the orthorhombic a direction from the high Tc superconductors Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BISCO-2212) is reported. The investigation has been extended to high and low temperatures for optimally doped crystals, to crystals with different doping levels and to the one layer compound Bi$_2$Sr$_2$CaCu$_2$O$_{6+\delta}$ (Bi-2201). The most striking feature is that both, the intensity of the diffuse scattering and the extent of the 2DSRO vary with doping as the critical temperature, $T_c$. These findings show that these short range ordering features are of importance for a better understanding of high Tc materials, at least those from the BISCO family.

10:24AM A9.00011 Low temperature specific heat in underdoped YBa$_2$Cu$_3$O$_7$ single crystals, HAI-HU WEN, YUE WANG, HONG GAO, LEI SHAN, National Lab for Superconductivity, Institute of Physics, CAS, Beijing, China — One single crystal of YBa$_2$Cu$_3$O$_7$ has been post-annealed into six different doping levels in the underdoped region with $T_c$ ranging from 30 K to 90 K. The low temperature specific heat has been measured on these samples down to 100 mK with magnetic field applied along c-axis and a-b plane. By subtracting the specific heat measured in these two different field directions, we have successfully removed the Schottky anomaly and obtained the field induced increase of the specific heat coefficient $\Delta C/H$ becomes smaller towards underdoping, indicating a larger nodal gap slope. The implications of our results on the mechanism of cuprate superconductors are discussed based on the Fermi arc picture of normal state. The YBCO single crystal was provided by Prof. Xin Yao at Shanghai Jiaotong University, China.
10:36AM A9.00012 Thermodynamic properties of cuprate superconductors: Singularities and Pseudogaps. JAMES STOREY, MacDiarmid Institute, Victoria University; JEFFERY TALLON, GRANT WILLIAMS, MacDiarmid Institute, Industrial Research Ltd — We have calculated the entropy and superfluid density of Bi-2212 from an ARPES-derived rigid energy dispersion and a model for the normal-state pseudogap. Their detailed doping and temperature dependence is found to closely mimic the experimentally measured data, thus indirectly validating the ARPES data. The doping level at which the Fermi level crosses a van Hove singularity (\(vHs\)) is determined and found to agree with that inferred from ARPES. The superfluid density is found to be linear in \(T\) at the vHs crossing. Surprisingly, the doping dependence of \(Tc\) seems to be unaffected by crossing the singularity.

10:48AM A9.00013 Confined vortex loops in superconductors with a magnetic core. MAURO DORIA, ANTONIO ROMAGUERI, UFRJ Rio de Janeiro Brazil, University of Antwerp Belgium, MILORAD MILOSEVIC, University of Bath UK; University of Antwerp Belgium, FRANCOIS PEETERS, University of Antwerp Belgium — A magnetic moment inside an extreme type II superconductor gives rise to confined vortex states in its neighborhood. We show how the presence of such states can be tracked down in the \(I-V\) characteristic curve, thus providing a simple method to their detection. The Lorentz force causes their growth and periodic evolution, passing through a long range ordered state (bulk) or an external vortex pair state (sub-micron particle). For a small magnetic moment there are exactly three confined vortex loops whereas for a large more elaborate vortex arrangements arise are possible. Their onset from the upper critical field core in sets of threes is proved to be energetically favorable over the growth of just one or two confined vortex loops independently of boundary conditions. All our results are derived in the context of the time-dependent and of the time-independent Ginzburg-Landau theory applied to a superconductor with periodic (bulk) and superconductor-insulator (sub-micron particle) boundary conditions, using three independent numerical methods.

Monday, March 5, 2007 8:00AM - 10:36AM — Session A10 DMP: Superconductivity: Electronic and Thermal Transport Properties
Colorado Convention Center Korbol 1E

8:00AM A10.00001 High Field Hall Effect and Resistivity in High-\(Tc\) \(La_{2-xSr_x}CuO_4\). FEDOR BALAKIREV, JONATHAN BETTS, ALBERT MIGLIORI, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, ICHIRO TSUKADA, YOICHI ANDO, Central Research Institute of Electric Power Industry, Komae, Tokyo 201-8511, Japan, GREGORY BOEBINGER, B. BALAKIREV, JONATHAN BETTS, ALBERT MIGLIORI, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, ICHIRO TSUKADA, YOICHI ANDO, Central Research Institute of Electric Power Industry, Komae, Tokyo 201-8511, Japan, GREGORY BOEBINGER, BALAKIREV, JONATHAN BETTS, ALBERT MIGLIORI, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, ICHIRO TSUKADA, YOICHI ANDO, Central Research Institute of Electric Power Industry, Komae, Tokyo 201-8511, Japan, GREGORY BOEBINGER, BALAKIREV, JONATHAN BETTS, ALBERT MIGLIORI, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, ICHIRO TSUKADA, YOICHI ANDO, Central Research Institute of Electric Power Industry, Komae, Tokyo 201-8511, Japan, GREGORY BOEBINGER.

8:12AM A10.00002 In-plane resistivity and Hall effect data of \(La_{2-xSr_x}CuO_4\) in high magnetic fields. SCOTT RIGGS, NHMFL / FSU, FEDOR BALAKIREV, ALBERT MIGLIORI, JON BETTS, NHMFL / LANL, GREG BOEBINGER, NHMFL / FSU, GENNA LOGVENOV, TONY BOLLINGER, IVAN BOZOVIĆ, BNL, NHMFL / BNL COLLABORATION — The effects of stoichiometry (Sr concentration in \(La_{2-xSr_x}CuO_4\) - LSCO) are of extreme interest in exploring the phase space of high-temperature superconductivity (HTS). Carrier doping in LSCO is determined by the Sr concentration rather than non-stoichiometric oxygen, thus controlling the carrier concentration in LSCO tends to be easier than in the other HTS cuprates. Nevertheless, precise control of Sr at a precision greater than 0.005 is extremely difficult using existing single crystal growth techniques. We use our unique MBE growth chamber to grow combinatorial thin films of LSCO with a uniform gradient of Sr concentration across a single substrate. Intense magnetic fields suppress superconductivity, revealing the underlying normal state to temperatures below 0.3K. We report the Hall effect and resistivity with an extremely fine \(\Delta x=0.0002\) Sr resolution in fields up to 60T.

8:24AM A10.00003 Low-temperature specific heat and thermal Hall conductivity in a vortex state of \(d\)-wave superconductors. ASHOT MELIKYAN, Materials Science Division, Argonne National Laboratory, OSKAR VAFEK, Florida State University and National High Magnetic Field Laboratory — We analyze the mixed state of thin \(La_{2-xSr_x}CuO_4\) film samples in magnetic field up to 60T. The Sr doping, \(x\), was varied between 0.08 and 0.22. The resistivity and Hall voltage were measured simultaneously by the Sr resolution in fields up to 60T.

8:36AM A10.00004 The Hall Number, Optical Sum Rule and Carrier Density for the \(t - t' - J\) Model. SRIRAM SHAstry, UCSC, Santa Cruz, CA, JAN HAERTER, UCSC — Mott Hubbard systems, epitomizing strong correlations and a sensitivity to half filling, display striking departures from band theory for many measurable. E.g. consider two quantities; the Hall constant \(RH\) and the optical conductivity sum rule \(\omega_p^2/8\). These are often inverted to give the carrier densities \(n_{H} \equiv 1/\rho_c RH\) and \(n_{OP} \equiv \frac{m}{4\pi q_e^2} \omega_p^2\). There is considerable difficulty in reconciling these with the, the "chemical" estimate of density in many High \(Tc\) systems[1]. We have argued previously[2] that the Hall constant is a manybody object, that need not scale simply with \(x\). In this work, we compute the variables \(n_{H}\) and \(n_{OP}\) for a \(t - t' - J\) model by using exact diagonalization of small clusters and different dopings \(x\). We calculate the Kubo formulas exactly for small clusters, and also the high frequency Hall constant for even larger systems, and obtain a strong dependence of these variables on the ratio \(t'/t\). We also comment on the departure from Luttinger’s theorem for the Fermi surface for these clusters, defining the same from the tower of excited states for a given wave vector for an added particle or hole. [1] W. Padilla et al., Phys. Rev. B 72, 060511(2005); [2] B. S. Shastry, B. I. Shraiman and R. R. P. Singh, Phys. Rev. Lett. 70, 2004(1993).

1NSF DMR-0408247
8:48AM A10.00005 Nernst effect as a probe of superconducting fluctuations in Nb0.15Si6.85. A. POURRET, H. AUBIN, J. LESUEUR, K. BEHNIA, Laboratoire de Physique Quantique(CNRS), ESPCI, 10 Rue Vauquelin, Paris, France. C. MARRACHE-KIKUCHI, L. BERGE, L. DUMOULIN, CNISM, IN2P3-CNRS,Bâtiment 108, 91405 Orsay, France — We present a study of the Nernst effect in thin films of the amorphous superconductor Nb0.15Si6.85. A finite Nernst signal was resolved at temperatures well above Tc, and at relatively high magnetic fields (1). In the zero-field limit and close to Tc, our results are in very good agreement with a simple relation derived from the theory by Ussishkin, Sondhi and Huse (2) for a two-dimensional superconductor. According to the theory, the magnitude of the Nernst signal generated by the fluctuating Cooper pairs depends only on the superconducting coherence length ξ. Far above Tc and/or in presence of a finite magnetic field, a departure from this relation is observed. Yet, even in this regime, the amplitude of the Nernst coefficient depends on a single length scale set by ξ and/or B. This observation allows to establish a phenomenological relation for the Nernst coefficient, for all magnetic fields and temperatures above Tc, which depends only on the size of the superconducting fluctuations set by ξ and/or B.


9:00AM A10.00006 On the heat current in the magnetic field: Nernst-ETtingshausen effect above the superconducting transition1, ANDREI SERGEEV, VLADIMIR MITIN, University at Buffalo, MICHAEL REIZER, 5614 Naiche Rd, Columbus OH — For maintaining gauge invariance in a magnetic field, the heat current operator should include the magnetic term. Taking this term into account, we revised calculations of the Nernst-ETtingshausen effect above the superconducting transition. We found that the fluctuations of the modulus of the order parameter do not change the particle-hole asymmetry (PHA) of the thermomagnetic effects in the fluctuation region are proportional to the square of PHA and, therefore, small. Magnetization currents in the electric field contribute to the charge and energy transfer, but not to the heat current. Only in this way, one can obtain the Nernst and ETtingshausen coefficients that satisfy to the Onsager relation. Large Nernst effect observed in the high-temperature cuprates requires vortex-like excitations due to the phase fluctuations, which are beyond the Gaussian-fluctuation theory.

1This work was supported by NYSTAR.

9:12AM A10.00007 Nernst effect and diamagnetism in a vortex liquid, DANIEL PODOLSKY, University of California at Berkeley, SRINIVAS RAGHU, Stanford University, ASHVIN VISHWANATH, University of California at Berkeley — When a superconductor is warmed above its critical temperature Tc, superconductivity is destroyed by fluctuations in the order parameter. These fluctuations are seen in a variety of experimental probes, including conductivity, diamagnetism, and the Nernst effect – the thermoelectric analogue of the Hall effect. In this talk we will discuss a regime in which superconductivity is destroyed by phase fluctuations arising from a dilute liquid of mobile vortices. The local superconducting correlations in this state lead to unusual properties, which are theoretically captured by a thermally fluctuating XY model in which amplitude fluctuations remain effectively frozen. We find that the Nernst effect and diamagnetic response differ dramatically from those arising from Gaussian fluctuations – in particular, a more rapid decay with temperature is obtained. We predict a rapid onset of Nernst effect at a temperature Tnuclei, and show that this scale tracks Tc rather than the pairing temperature. We predict a close quantitative connection between the diamagnetism – the ratio of magnetization to transverse thermoelectric conductivity αxy reaches a universal value at high temperatures. We compare our results to Nernst effect measurements on the underdoped cuprates, and interpret these results in terms of a dilute vortex liquid over a fairly wide temperature range above Tc.

9:24AM A10.00008 Anomalous quasiparticle thermal transport in the superconducting state of ultra pure URu2Si2 single crystals, YUICHI KASAHARA, T. IWASAWA, T. SHIBAUCHI, Kyoto Univ., Y. MATSUDA, Kyoto Univ., Institute for Solid State Physics, Univ. of Tokyo, K. BEHNIA, Laboratoire de Physique Quantique, ESPCI, T. D. MATSUDA, Y. HAGA, Japan Atomic Energy Agency (JAEA), Y. ONUKI, Osaka Univ., JAEA — In heavy fermion superconductor URu2Si2, although it is believed that superconductivity in this material (Tc ~ 1.5 K) is unconventional, details of the superconducting gap structure are still unknown. To investigate the quasiparticle transport in the superconducting state of URu2Si2, the thermal conductivity κ is measured in pure single crystals with residual resistivity ratio ~ 600. In zero field, κ/T shows a steep increase below Tc, indicating that the quasiparticle mean free path is strongly enhanced in the superconducting state. A finite residual term of κ/T as T → 0 is clearly resolved, together with a T3 dependence at very low temperatures. With applying magnetic field, thermal conductivity grows rapidly at low magnetic fields, and exhibits a √T dependence. These results strongly indicate a presence of line nodes in the superconducting gap function. We found that κ/T exhibits a sudden drop at upper critical field, which has never been observed in any superconductors. We discuss this unusual behavior of thermal conductivity in the context of anomalously large ωcτ (τ > 1) and giant magnetoresistance observed in this material.

9:36AM A10.00009 Low Temperature Heat Transport in the superconducting skutterudite PrOs4Sb12:2, Evidence for nodes in the superconducting gap, ROBERT HILL, University of Waterloo, BRIAN MAPLE, University of California San Diego, SHIYAN LI, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, Université de Sherbrooke — Thermal conductivity measurements were performed on single crystal samples of the superconducting skutterudite material PrOs4Sb12:2 both as a function of temperature and as a function of magnetic field applied perpendicular to the heat current. In zero magnetic field we find clear evidence for residual electronic conduction as the temperature increases below Hc1, increasing by a factor 10 in 100 mT (~ 0.05 Hc2). This is consistent with a semi-classical theory based on a Doppler-shift of the quasiparticle spectrum through coupling to the superfluid flow around magnetic vortices.

9:48AM A10.00010 Probing the nodal metal in LBCO with heat transport, RAMZY DAOU, LOUIS TAILLEFER, Université de Sherbrooke, QIANG LI, GENDA GU, Brookhaven National Laboratory — The cuprate superconductor La2−xBaxCuO4 (LBCO) has a near-zero minimum in the superconducting transition temperature at x = 1/8. This is accompanied by the emergence of static one-dimensional spin and charge ordering in “stripes” [1]. Spectroscopic measurements at the same doping in the normal state have shown that a gap with d-wave symmetry is present in the single particle spectrum, and the opening of a gap in the density of states of the superconducting ground state by phase fluctuations suppressing Tc while leaving gapped but “uncondensed” Cooper pairs and nodal quasiparticles. We present measurements of the thermal conductivity of LBCO at very low temperature in both superconducting and field-induced nodal metal states. [1] P. Abrahmson et al., Nature Physics 1, 155 (2005) [2] T. Valla et al., Science. 10.1126/1134742 (2006)

10:00AM A10.00011 One Dimensional Superconducting Transition in Quasi-Two-Dimensional Stripes, MATTHEW BELL, ANDREI SERGEEV, ALEKSANDR VEREVKIN, University at Buffalo — We investigate the nature of the superconducting transition in NbN ultrathin nano stripes where the thickness of the stripe (4 nm) is about or less then the coherence length, and the width (100 nm) is significantly larger then the coherence length. It is well known that in micro stripes the resistive state below the Berezinskii-Kosterlitz-Thouless transition is produced by disordered vortex-antivortex pairs. However, our data clearly demonstrates that in such structures the resistive state is formed due to one-dimensional phase slip centers (PSCs) at low current densities. Our analysis shows that the resistive state is actually a result from the competition between the PSCs and two-dimensional vortices. At low currents, the PSC mechanism prevails over the contribution from vortices over a broad temperature range. At higher currents, current induced unbinding of vortex-antivortex pairs contributes the most to resistivity, however this effect is limited by electron heating. From this analysis we will develop a current-temperature phase diagram for superconducting nano stripes.
10:12AM A10.00012 Thermal Expansion at the Superconducting Phase Transition in Nb\textsuperscript{1}.  
RICHARD K. BOLLINGER, JOHN J. NEUMEIER, Montana State University, CARLOS A.M. DOS SANTOS, Escola de Engenharia de Lorena, Montana State University, HUGO R.Z. SANDIM, Escola de Engenharia de Lorena — Thermal expansion is an important thermodynamic quantity that is difficult to measure with sufficient precision to observe electronic phase transitions such as the normal to superconducting transition. Thermal expansion data will be presented on the superconducting to normal phase transition of Nb (\(T_c = 9.27\) K), obtained with a novel quartz dilatometer cell. Surprisingly, only one prior report of this measurement has been published.\textsuperscript{2} This report does not clearly show the predicted jump at \(T_c\). Thermal expansion data can be used to compute the pressure derivative of \(T_c\), and this analysis will be presented. \textsuperscript{*} White, G.K., \textit{Cryogenics} 2, 292 (1962).

\textsuperscript{1}This material is based upon work supported by the US DOE (DE-FG-06ER46269) and NSF (DMR-0504769).

10:24AM A10.00013 On the Nature of the Superconducting Transition in YBCO\textsuperscript{1}. M. YETHIRA\textsuperscript{2}, Bragg Institute, ANSTO, S.J. CROWE, D. MCK. PAUL, University of Warwick, D.K. CHRISTEN, ORNL, M. ARAI, Japan Atomic Energy Agency, T. YOKO, Institute of Materials Structure Science, KEK, L. PORCAR, P.D. BUTLER, NCNR, NIST — In the high-Tc superconductor YBCO, a transition was observed from a hexagonal FLl at low magnetic field (parallel to the c-axis) to a square configuration at high fields. Also seen was a rapid decrease in the Bragg intensity at low temperature (T). It has been the general belief that both the symmetry change and the T-dependence behaviour was due to the d-wave nature of high-Tc superconductivity. However, we observed that the fall-off in intensity with increasing temperature depended on the strength of the applied external field and that excellent fits to this T-dependence could be obtained by simply multiplying the temperature dependence of the familiar Ginzburg-Landau two-fluid model, appropriate for high-kappa materials conventional superconductors, by an exponential factor \(\exp(-aT)\), with the field-dependent variable ‘a’ being the only free parameter. The impact of these observations on the symmetry of the order parameter will be discussed.

\textsuperscript{2}Previous Affiliation: Oak Ridge National Laboratory

Monday, March 5, 2007 8:00AM - 11:00AM — Session A11 DMP: Magnetic Phase Transitions Colorado Convention Center Korbel 1F

8:00AM A11.00001 Competing magnetic fluctuations in \(\text{Sr}_x\text{Ru}_2\text{O}_7\) probed by Ti doping. DAVID FOBES, J. HOOPER, M. ZHOU, N. DANG, Z.Q. MAO, Tulane University, USA, M.H. FANG, C.M. FENG, Z.A. XU, Zhejiang University, China, M.H. YU, C.J. O’CONNOR, University of New Orleans, USA, G.J. XU, N. ANDERSEN, Riso National Laboratory, Denmark, M. SÁLAMON, University of Illinois at Urbana-Champaign, USA — The layered ruthenate \(\text{Sr}_x\text{Ru}_2\text{O}_7\) shows itinerant metamagnetic quantum criticality which has been cited as a textbook example. In this talk we report the effect of nonmagnetic Ti\textsuperscript{4+} impurities on the electronic and magnetic properties of this material. Small amounts of Ti suppress the characteristic peak in magnetic susceptibility near 16 K and result in a sharp upturn in specific heat. The metamagnetic quantum phase transition and related anomalous features are quickly smeared out by small amounts of Ti. These results provide strong evidence for the existence of competing magnetic fluctuations in the ground state of \(\text{Sr}_x\text{Ru}_2\text{O}_7\). Ti doping suppresses the low temperature antiferromagnetic interactions that arise from Fermi surface nesting, leaving the system in a state dominated by ferromagnetic fluctuations.

8:12AM A11.00002 Effect of Magnetic Field on Electronic Nematic Order in a Bilayer System: Application to \(\text{Sr}_3\text{Ru}_2\text{O}_7\). CHRISTOPH PUETTER, HYEONJIN DOH, HAE-YOUNG KEE, Department of Physics, University of Toronto, Toronto, Ontario, Canada MSS 1A7 — Recent experiments on the bilayer compound \(\text{Sr}_3\text{Ru}_2\text{O}_7\) suggest the existence of an electronic liquid-crystal phase. A possible explanation for the unusual behavior observed in this material is provided by an electronic nematic theory. Within this framework, a bilayer system undergoes multiple phase transitions and exhibits strong transport anisotropy. The model also incorporates an external in-plane magnetic field to study the effect on metamagnetic transitions and anisotropic transport. Details of our numerical calculations will be presented.

8:24AM A11.00003 Magnetic Phase Transition and Magnetic Structure of \(\text{Ca}_3\text{Ru}_2\text{O}_7\). Z. QU, J. PENG, T.J. LIU, F. ETIENNE, D. FOBES, Z.Q. MAO, Physics Department, Tulane University, New Orleans, LA 70118, W. BAO, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 — \(\text{Ca}_3\text{Ru}_2\text{O}_7\) shows exciting physical properties, including a bulk spin-valve behavior and orbital ordering.\textsuperscript{[1–3]} We have investigated the magneto-transport properties and the magnetic structure of this material using high-quality \(\text{Ca}_3\text{Ru}_2\text{O}_7\) single crystals grown by a floating-zone (FZ) method. From magnetoresistivity measurements, we observe that the previously reported metamagnetic transition at ~6T for \(H/\alpha\) axis consists of two separate transitions occurring at 5.9 and 6.5T, respectively. The first transition is extremely sharp with the transition width less than 1 Gauss, corresponding to the bulk spin-valve behavior, while the second transition has a finite width which is likely associated with the change of orbital polarization. Our elastic neutron scattering measurements on FZ-grown \(\text{Ca}_3\text{Ru}_2\text{O}_7\) single crystals confirm the magnetic structure suggested by previous works.\textsuperscript{[2,4]} i.e., the magnetic moments align ferromagnetically within the double layers and antiferromagnetically between the double layers. 1. X.N. Lin et al., Phys. Rev. Lett., 95, 017203 (2005). 2. D.J. Singh and S. Auluck, Phys. Rev. Lett., 96, 097203 (2006). 3. J.F. Karpus, et al., Phys. Rev. Lett., 93, 167205 (2004). 4. Y. Yoshida, et al., Phys. Rev. B, 72, 054412 (2005).

8:36AM A11.00004 Specific Heat of \((\text{Ca}_{1-x}\text{Sr}_x)\text{Ru}_2\text{O}_7\) Single Crystals\textsuperscript{1}. V. VARADARAJAN, S. CHIKARA, V. DURAIRAJ, X.N. LIN, G. CAO, J.W. BRILL, University of Kentucky — We have measured the specific heat of crystals of \((\text{Ca}_{1-x}\text{Sr}_x)\text{Ru}_2\text{O}_7\) using ac- and relaxation-time calorimetry. Special emphasis was placed on the characterization of the Neél (\(T_N\approx56\) K) and structural (\(T_c = 48\) K) phase transitions in the pure, \(x=0\) material. While the latter is believed to be first order, detailed measurements under different experimental conditions suggest that all the latent heat (with \(L \sim 0.3\) R) is being captured in a broadened peak in the effective heat capacity. The specific heat has a mean-field-like step at \(T_N\), but its magnitude (\(\Delta c_p \sim R\)) is too large to be associated with a conventional itinerant electron (e.g. spin-density-wave) antiferromagnetic transition, while its entropy is too small to be associated with full ordering of localized spins. The \(T_N\) transition broadens with Sr substitution while its magnitude decreases slowly. On the other hand, the entropy change associated with the \(T_c\) transition decreases rapidly with Sr substitution and is not observable for our \(x=0.58\) sample.

\textsuperscript{1}Supported by NSF, grants DMR-0400938 and DMR-0552267
8:48AM A11.00005 In-plane anisotropy of magnetoresistivity of tri-layered ruthenate Sr$_3$Ru$_2$O$_{10}$ . Z.Q. MAO, M. ZHOU, D. FOBES, Tulane University, H.Q. YUAN, M. SALAMON, University of Illinois at Urbana-Champaign — The tri-layered ruthenate Sr$_3$Ru$_2$O$_{10}$ exhibits intriguing magnetic properties: its ferromagnetic transition at $T_c \approx 105$ K is followed by an additional magnetic phase transition at $T' \approx 50$ K [1,2]. Below $T'$, a first order magnetic transition is induced by a magnetic field applied in the plane. We have recently measured the in-plane angular dependence of magnetoresistivity of this material at various magnetic fields and temperatures. Our data reveal that the in-plane anisotropy of magnetoresistivity undergoes a transition from two-fold to four-fold symmetry across the metamagnetic transition of Sr$_3$Ru$_2$O$_{10}$. Such a transition can be well interpreted in terms of a multiple-band effect which involves the coexistence of ferromagnetic and metamagnetic bands.


9:00AM A11.00006 Long Range Order in Orbital Model , WENLONG YOU, GUANGSHAN TIAN, HAIQING LIN, Department of Physics, The Chinese University of Hong Kong, Shatin, N. T., Hong Kong — We investigate the existence of Néel type long range order (LRO) in an orbital model which is highly anisotropic and frustrated. The model originated from magnetic materials such as LaMnO$_3$ where orbital degrees of freedom play important role. In the system described by the two-fold degenerate $e_g$ orbitals, due to the Kugel-Khomskii superexchange, the orbital degrees of freedom are represented by quantum pseudo-spin 1/2 operators. By applying the reflection-posivity method developed by Dyson, Lieb, and Simon, and adopting appropriate numerical variational method to obtain good estimations on the energy density and correlation functions, we are able to rigorously prove the existence of long range order in this orbital model on the square lattice.

9:12AM A11.00007 Orbital order and spin waves in the Kugel-Khomskii model, TAMAR Pereg-BARNEA, WEI-CHENG LEE, ALLAN MACDONALD, University of Texas at Austin — The Kugel-Khomskii model, introduced in the seventies, attempts to describe transition metal oxides in which orbital degeneracy plays an important role in ground state properties. The model provides a qualitative description of pseudocubic perovskites like LaTiO$_3$ and YTiO$_3$ in which the three $t_{2g}$ d-orbitals are thought to be active at low energy. We investigate the cubic $t_{2g}$ Kugel-Khomskii model in the limit of strong electron-electron interaction (on-site Hubbard U). We use perturbation theory with small hopping parameter (t/U) to derive an effective large pseudospin Hamiltonian with 6 degrees of freedom on each site (2 spins X 3 orbitals). In this model the $t_{2g}$ orbital structure combined with cubic symmetry leads to hoppings that depend on both the orbital label and the bond direction. We find the classical (mean-field) ground state manifold systematically and derive a spin wave theory to account for quantum fluctuations. The theory proceeds beyond leading order in order to capture the coupling between the spin and orbital degrees of freedom of the system. This approach leads to better understanding of the quantum-mechanical ground state, its energy and symmetries.

$^1$Work supported by NSERC, the Welch Foundation and the NSF

9:24AM A11.00008 Optical spin waves in magnetite, R.J. MCQUEENEY, Iowa State University, M. YETHIRAJ, ANSTO, W. MONTFROOIJ, Missouri University, S. CHANG, Ames Laboratory, T.G. PERRING, Rutherford Appleton Laboratory, P. METCALF, J.M. HONIG, Purdue University — For the last 70 years, the microscopic origin of the Verwey transition in magnetite (Fe$_3$O$_4$) was thought to be charge-ordering, although this has been disputed of late, bringing renewed interest in this system. The spin structure of magnetite contains two different iron sites; A (stable valence, Fe$^{3+}$) and B (mixed valence, Fe$^{2.5+}$), with charge ordering of Fe$^{2.5+}$/Fe$^{3+}$ species occurring on the B-site. As the spin waves are expected to be sensitive to charge ordering, the optical spin waves were measured above and below the Verwey transition by inelastic neutron scattering. The optical spin waves propagating on the A-site sublattice ($\sim$115 meV) are unchanged at the transition. The spin waves propagating on the B-site sublattice ($\sim$75 meV) are $\sim$5 meV stiffer and broader in the metallic phase. The results are interpreted as evidence of B-site double exchange in the metallic phase.

9:36AM A11.00009 Electronic Raman scattering in Magnetite, LEV GASPAROV, University of North Florida, G. GUNTERODT, II. Physikalisches Institut, RWTH-Aachen, Germany, K.-Y. CHOI, NHMFL - Tallahassee, FL, USA, H. BERGER, L. FORRO, EPFL-Lausanne, Switzerland — Raman spectra of optimally doped magnetite (Fe$_3$O$_4$) single crystals reveal broad electronic background extending up to 900 wavenumbers ($\sim$110 meV). Redistribution of this background is observed when sample is cooled below the Verwey transition temperature ($T_V = 123K$). In particular, spectra of the low temperature phase show diminished background below 300 wavenumbers followed by an enhancement of the electronic background between 300 and 400 wavenumbers with subsequent decrease of the background below 400 wavenumbers. Such redistribution may be assigned to an opening of the charge gap of the low temperature phase show diminished background below 300 wavenumbers followed by an enhancement of the electronic background between 300 and 400 wavenumbers. The value of the gap is within the range of the photoemission data on freshly fractured magnetite sample.

$^2$This work was supported by the Alexander von Humboldt Foundation, Research Corporation Cottrell College Science award #CC0130, Petroleum Research Fund award #40926-GB10.

9:48AM A11.00010 Resonant x-ray scattering of the Bi$_{1-x}$Sr$_x$MnO$_3$ (x<0.5) charge-ordered phases, JOAQUIN GARCIA, GLORIA SUBIAS, M.C. SANCHEZ, ICMA, CSIC-Universidad de Zaragoza, Spain, PREMEK BERAN, J. L. GARC´ıA-MUNOZ, ICMA, CSIC, Bellaterra Spain, M. NEVRIVA, Institute of Chemical Technology, Prague, Czech Republic — Charge-ordered orbital ordering (COOO) in Bi$_{1-x}$Sr$_x$MnO$_3$ (x=0.3, 0.5) have been studied by resonant x-ray scattering (RXS) at the Mn K edge. Strong resonances were observed at the Mn K-edge for weak superstructure (h00), (00k) and forbidden (h/200), (0k/20) reflections with k odd in the ab plane setting (bmmm setting) in both single crystals. Additional (h0k) and (hk/20) with k odd have also been studied. The azimuth angle and polarization dependence of the resonant intensity for this set of reflections point out to a structural transition at the $T_{COO}$ that stabilizes an checkerboard ordering of two non-equivalent Mn atoms with different local geometrical structures and a very small change between for x=0.5 and x=0.3 compounds. We can conclude that A$_1$-$\delta$B$_\delta$MnO$_3$ tends to order in a checkerboard pattern independently of the nature of the A and B atoms and for x even far from 0.5. Furthermore, the electronic states of the two non-equivalent Mn atoms are far from the ionic (+3 and +4) species.

10:00AM A11.00011 Effect of Charge Ordering on Phonon Spectra of La$_{1-x}$Sr$_{2/3}$FeO$_{3-x}$, JIE MA, S. CHANG, J.-Q. YAN, Ames Lab., Dept. of Phys. & Astro., Iowa State U, Ames, IA, 50011, F. TROUW, M. HEHLEN, LANL, R. J. MCQUEENEY, Ames Lab., Dept. of Phys. & Astro., Iowa State U, Ames, IA, 50011, AMES LAB., DEPT. OF PHYS. & ASTRO., IOWA STATE U, Ames, IA, 50011 TEAM, LANL COLLABORATION — La$_{1/3}$Sr$_{2/3}$FeO$_{3-x}$ (LSFO) compounds are reported to have an unusual magnoeto-structural transition at low temperatures. Below $\sim$210 K, it is proposed that charge disproportionation occurs according to 3Fe$^{3.67+}$+ $=\rightarrow$2Fe$^{3+}$+Fe$^{4+}$, and the different iron valences order in the pattern 3+, 3+, 5+ along the body diagonal [111]. Simultaneously, LSFO undergoes antiferromagnetic ordering and a slight distortion in crystal structure from cubic to rhombohedral. Inelastic neutron scattering was used to determine the effect of the charge ordering on the phonon spectra. We find that the high frequency oxygen phonons ($\sim$80 meV) soften above the transition by several meV. The result and relationship between the charge ordering and the phonon softening are discussed.
we observe the electrical generation of a transverse spin current, which can drive spin polarization nearly 40 microns into a transverse channel. Using a model transport and electron systems. More recently, we investigate spin currents generated by the spin Hall effect in GaAs structures that distinguish edge effects from spin polarization and the spin Hall effect. Current-induced spin polarization results in spins being polarized by the internal magnetic field arising from spin-orbit and quantum logic. Recently we have explored two mechanisms for electrically generating spin polarization in non-magnetic materials: current-induced spin density wave, the influence of antiferromagnetic domain walls, and the existence of more than one scattering time. \[1\] “Quantum phase transition in a common metal”, A. Yeh, Y-A. Soh, J. Brooke, G. Aeppli, T. F. Rosenbaum, and S. M. Hayden, Nature (London) 419, 459 (2002).

We thank the Beckman Foundation for supporting the project.

10:48AM A11.00015 Thermomagnetic Studies of $K_2NaCrO_3$ \(^1\), SARITHA NELLUTLALA, National High Magnetic Field Laboratory, MEKHALA PATI, Florida State University, KWANYONG CHOI, Florida State University and NHMFL, YOUNJUNG JOO, National High Magnetic Field Laboratory, NAARESH DALAL, Florida State University and NHMFL, LUIS BALICAS, JOHAN VAN TOL, National High Magnetic Field Laboratory, DANIEL PAJEROWSKI, BYoung HEE MOON, Yoonseok Lee, Mark Meisel, Yasumasa Takano, University of Florida — There has been renewed interest in the search for new model quantum spin systems that can exhibit BEC of magnons. $K_2NaCrO_3$ is one of the simplest spin systems available since $S = 1/2$ and $I = 0$. Specific heat ($C_p$) measurements indicate that this material orders antiferromagnetically at $T_N \approx 1.7$ K in zero-field \([1]\). Application of an external magnetic field pushes the $C_p$ maximum to lower temperatures. Torque and AC susceptibility measurements show that the transition temperature is rapidly suppressed around 7.4 T, with no hysteretic behavior, implying the presence of a quantum phase transition. Measurements are underway to map the phase boundary in the $T \rightarrow 0$ K, $B \sim 7.4$ T region and extract the critical exponent ($\alpha$) from the relation $k_B T_\alpha \approx (B_\alpha - B)^\alpha$. \[1\] B. Cage, N. S. Dalal, Chem. Mater. 13, 881 (2001).

1Supported by NASA Grant # NNG05GQ35G (NSD), NHMFL-IHRP (YT), NSF DMR-0305371 and DMR-0239483 (YL).

Monday, March 5, 2007 8:00AM - 11:00AM — Session A12 GMAG DMP FIAP: Focus Session: Spin Hall Effect — Colorado Convention Center Korbel 3C

8:00AM A12.00001 Generating Spin Currents in Semiconductors with the Spin Hall Effect \(^1\). DAVID AWSCHALOM\(^2\), Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — There is a growing interest in exploiting electron spins in semiconductor nanostructures for the manipulation and storage of information in emergent technologies based upon spintronics and quantum logic. Recently we have explored two mechanisms for electrically generating spin polarization in non-magnetic materials: current-induced spin polarization and the spin Hall effect. Current-induced spin polarization results in spins being polarized by the internal magnetic field arising from spin-orbit coupling, and the spin Hall effect refers to the generation of a spin current transverse to a charge current in the absence of an applied magnetic field. Recent measurements in $ZnSe$ reveal that both of these effects are robust to room temperature\[^{11}\]. Although spin current is difficult to measure directly, the spin Hall effect creates spin accumulation at the edges of a channel which has been measured in bulk epilayers of n-doped semiconductors and in two-dimensional hole and electron systems. More recently, we investigate spin currents generated by the spin Hall effect in GaAs structures that distinguish edge effects from spin transport\[^{11}\]. We fabricate mesas with transverse channels to allow spins to drift into regions in which there is minimal electric current, and the spin Hall effect refers to the generation of a spin current transverse to a charge current in the absence of an applied magnetic field. Recent measurements in $ZnSe$ reveal that both of these effects are robust to room temperature\[^{11}\]. Although spin current is difficult to measure directly, the spin Hall effect creates spin accumulation at the edges of a channel which has been measured in bulk epilayers of n-doped semiconductors and in two-dimensional hole and electron systems. More recently, we investigate spin currents generated by the spin Hall effect in GaAs structures that distinguish edge effects from spin transport\[^{11}\].

1Work supported by DARPA, NSF and ONR.

2Work performed in collaboration with V. Sih, W. H. Lau, R. C. Myers, V. R. Horowitz and A. C. Gossard.


8:36AM A12.00002 Persistent Spin Helix — BOGDAN BERNIEV, Princeton University, JOE OREINSTEIN, UC Berkeley, SHOU-CHENG ZHANG, Stanford university — Spin-orbit coupled systems generally break the spin rotation symmetry. However, for a model with equal Rashba and Dresselhaus coupling constant (the RoD model), and for the $\{110\}$ Dresselhaus model, a new type of SU(2) spin rotation symmetry is discovered. This symmetry is robust against spin-independent disorder and interactions, and is generated by operators whose wavevector depends on the coupling strength. It renders the spin lifetime infinite at this wavevector, giving rise to a Persistent Spin Helix (PSH). We obtain the spin fluctuation dynamics at, and away, from the symmetry point, and suggest experiments to observe the PSH.
8:48AM A12.00003 Topological Insulators in Three Dimensions1, LIANG FU, CHARLES KANE, EUGENE MELE, University of Pennsylvania — We study three dimensional generalizations of the quantum spin Hall (QSH) effect. Unlike two dimensions, where the QSH effect is distinguished by a single $Z_2$ topological invariant, in three dimensions there are 4 invariants distinguishing 16 "topological insulator" phases. There are two general classes: weak (WTI) and strong (STI) topological insulators. The WTI states are equivalent to layered 2D QSH states, but are fragile because disorder continuously connects them to band insulators. The STI states are robust and have surface states that realize the 2+1 dimensional parity anomaly without fermion doubling, giving rise to a novel "topological metal" surface phase. We show that the $Z_2$ invariants can be easily determined for systems with inversion symmetry. This allows us to predict specific materials are STIs, including semiconducting alloy Bi$_{1-x}$Sb$_x$ as well as α-Sn and HgTe under uniaxial strain.

1This work was supported by NSF grants DMR-0605066

9:00AM A12.00004 Skew-scattering contribution in Rashba-type 2D systems with short-range scalar impurity potential, MARIO F. BORUNDA, Texas A&M University, TAMARA NUNNER, THOMAS LUECK, Freie Universität Berlin, NIKOLAI SINITSYN, Los Alamos National Lab, CARSTEN TIMM, University of Kansas, TOMAS JUNGWIRTH, Institute of Physics ASCR, JAIRO SINNOVA, Texas A&M University — There is a renewed interest in the anomalous Hall effect (AHE) motivated by the fabrication of materials that are both ferromagnetic and semiconducting, diluted magnetic semiconductors (DMS). Experimental and theoretical studies have shown that the skew-scattering contribution can have a dominant role in magnetotransport, especially in the low-impurity-concentration limit. The Hamiltonian describing Rashba-type systems is sufficiently simple to allow analytical solutions, yet it has the features of a typical DMS: (1) spin-orbit coupling, (2) more than one band with momentum-dependent Berry’s curvature, and (3) it allows for both intra- and inter-band scattering on impurities. We estimate skew-scattering contribution to two-dimensional Rashba-coupled systems in the leading order of expansion in disorder strength. We consider short-range disorder potentials and derive the general formula for arbitrary spin-orbit coupling through a high-order Born approximation.

9:12AM A12.00005 Low field phase diagram of spin-Hall effect in the mesoscopic regime, ZHENHUA QIAO, WEI REN, Department of Physics, The University of Hong Kong, Hong Kong, China, JIAN WANG, Department of Physics and the Center of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China, HONG GUO, Center for the Physics of Materials & Department of Physics, McGill University, Montreal, PQ, Canada — When a mesoscopic two dimensional four-terminal Hall cross-bar with Rashba and/or Dresselhaus spin-orbit interaction (SOI) is subjected to a perpendicular uniform magnetic field $B$, both integer quantum Hall effect (IQHE) and mesoscopic spin-Hall effect (MSHE) may exist when disorder strength $W$ in the sample is weak. We have calculated the low field ‘phase diagram’ of MSHE in the $(B,W)$ plane for disordered samples in the IQHE regime. For weak disorder, MSHE conductance $G_{sH}$ and its fluctuations $rmsG_{sH}$ vanish identically on even numbered IQHE plateaus, they have finite values on odd numbered plateaus induced by SOI, and they have values $G_{sH} = 1/2$ and $rmsG_{sH} = 0$ on those odd numbered plateaus induced by Zeeman energy. For moderate disorder, the system crosses over into a regime where both $G_{sH}$ and $rmsG_{sH}$ are finite. A larger disorder drives the system into a chaotic regime where $G_{sH} = 0$ while $rmsG_{sH} = 0$ is finite. Finally at large disorder both $G_{sH}$ and $rmsG_{sH}$ vanish. We present the physics behind this ‘phase diagram’.

9:24AM A12.00006 Quantum spin Hall phase and surface spin current in Bi and Sb, SHUICHI MURAKAMI, Department of Applied Physics, University of Tokyo — In the quantum spin Hall (QSH) phase, the bulk is gapped while edge states are gapless and carry spin currents. Experimental studies for the QSH phase are carried out. To search for candidates of the 2D QSH phase, we relate the spin Hall conductivity in insulators with magnetic response of the orbital magnetization to the Zeeman field. In this respect, bismuth is promising since it is a strong diamagnet enhanced by spin-orbit coupling. For a 2D (111)-bilayer bismuth, we calculate the $Z_2$ topological number, the band structure for the strip geometry, the spin Chern number, and the parity at the time-reversal symmetric wavenumbers. We predict that the (111)-bilayer bismuth will be a QSH phase [1]. On the other hand, by spin-orbit coupling through a high-order Born approximation.

9:36AM A12.00007 Mesoscopic Spin Hall Effect, PHILIPPE JACQUOD, University of Arizona, INANC ADAGIDELI, University of Regensburg, Germany, JENS BARDARSON, University of Leiden, The Netherlands — We investigate the spin Hall effect in ballistic chaotic quantum dots with spin-orbit coupling. We show that a longitudinal charge current can generate a pure transverse spin current. While this transverse spin current is generically nonzero for a fixed sample, we show that when the spin-orbit coupling time is short compared to the mean dwell time inside the dot, it fluctuates universally from sample to sample or upon variation of the chemical potential with a vanishing average. For a fixed sample configuration, the transverse spin current has a finite typical value $\propto e^2V/h$, proportional to the longitudinal bias $V$ on the sample, and corresponding to about one excess open channel for one of the two spin species. We discuss spin current correlations and noise.

9:48AM A12.00008 Spin torque contribution to the frequency dependent spin Hall conductivity in spin-orbit coupled systems, A. WONG-LOPEZ, F. MIRELES, J.A. MAYTORENA, C. LOPEZ-BASTIDAS, Centro de Ciencias de la Materia Condensada-UNAM — The spin Hall effect in spin-orbit coupled systems has lately attracted great attention. Since the electron spin is not a conserved quantity in spin-orbit coupled systems, the conventional form for the spin current operator turn out to be ill-defined. A fundamental issue is then a proper definition of spin current in such systems. Recently J. Shi et. al. [1] introduced an unambiguous and proper definition of spin current which adds to the conventional part, a spin source term (spin torque) associated to the spin precessional motion. In this work, using the linear response Kubo formalism, and employing the new definition for the spin current operator, we study the frequency dependent spin Hall conductivity for a two dimensional electron gas in the presence of Rashba and Dresselhaus spin-orbit coupling. We show that the optical spectrum of the charge and spin conductivity changes dramatically when the proper definition is used, as new and strong resonances appears. It is shown that the spin torque contribution to the spin Hall conductivity clearly dominates over the conventional part. These results may encourage experimentalists to measure the spin Hall current and/or spin accumulation in the frequency domain in such systems, as to establish the vality of the new definition of the spin current operator. [2] J. Shi, P Zhang, D. Xiao and Q Niu, Phys Rev. Lett 96, 076604 (2006)

10:00AM A12.00009 ABSTRACT WITHDRAWN —
10:12AM A12.00010 Search for the Persistent Spin Helix in a 2-Dimensional Electron Gas. J.D. KORALEK, C.P. WEBER, J. ORENSTEIN, Lawrence Berkeley National Laboratory, B.A. BERNEVIG, S.-C. ZHANG, Stanford University, S. MACK, J. STEPHENS, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — The persistent spin helix is an infinitely long-lived helical spin density wave that is predicted to occur in 2-dimensional electron systems with equal-strength Rashba and Dresselhaus spin-orbit coupling [Bernevig et al., cond-mat/0606196]. The infinite lifetime of the helix would result from the combined effects of diffusion and precession in the spin-orbit effective field. These effects would also greatly enhance the lifetime of spin excitations at the helix wave vector in systems where Rashba ≠ Dresselhaus. We use the transient spin grating technique to search for this effect in GaAs quantum wells. In these experiments, two non-collinear, orthogonally polarized pump pulses from a Ti:Sapphire oscillator generate a holographic spin grating in the interference region on the sample. The subsequent decay of the spin grating is monitored by diffraction of a time-delayed probe pulse. The wave vector of the spin grating can be tuned by varying the angle between the interfering pump beams, making this technique ideally suited for observing the persistent spin helix.

1Supported through NSF grants DMR-0342832, DMR-0305223, and by DOE contract DE-AC03-76SF00515.

10:24AM A12.00011 Berry Curvature and the $Z_2$ Topological Invariants of Spin-Orbit-Coupled Bloch bands. F. D. M. HALDANE, Princeton University — The (“anomalous”) integer quantum Hall effect can occur in non-interacting models of band insulators with broken time-reversal- $[T^-]$symmetry where the sum of Chern invariants of occupied bands of Bloch states is non-zero. These topological invariants can be computed from the zeroes of certain functions in the Brillouin zone (BZ), but have a simpler formulation as BZ-integrals of Berry curvature. Recently, Kane and Mele found that $T^-$-invariant 2D systems with strong spin-orbit coupling possess a “$Z_2^+$” (+ or $-$) analog of the Chern invariant, which they formulated in terms of zero-counting arguments (3D generalizations have also been found). I give an alternate formulation in terms of Berry-curvature integrals, in the case that spatial-inversion- $[J^-]$symmetry is broken, but $T^-$-symmetry is not. In 2D, such bands generically form a genus-5 2-manifold, with antipodal points paired by Kramers degeneracy: the $Z_2$ invariant is obtained by integration over a Kramers-distinct half-manifold; the 3D case is similar. I also discuss the case of doubly-degenerate bands with unbroken $J^-$-symmetry: despite recent suggestions, it does not appear that the $Z_2^-$ invariant of such systems can be obtained purely from knowledge of the parity quantum numbers at $J^-$-invariant points in the BZ.

1Supported by NSF MRSEC DMR-0213706.

10:36AM A12.00012 Quantum Spin Hall Effect in HgTe in a Magnetic Field. TAYLOR HUGHES, Stanford University, ANDREI BERNEVIG, Princeton University, SHOU-CHENG ZHANG, Stanford University — Recently, the quantum spin Hall effect has been proposed in HgTe quantum wells. It has been shown that this system exhibits the quantum spin Hall effect and the Hamiltonian is analogous to two copies of the quantum anomalous Hall effect. Here we examine the features of this system in a strong magnetic field. We use an analytic transfer matrix formalism to study the system on a lattice in a strip geometry in the presence of a strong perpendicular magnetic field. We characterize the bulk band structure and edge states for various applied field strengths and discuss possible experimental signatures of the quantum spin Hall effect. We also discuss possible discrepancies between the continuum and lattice picture.

10:48AM A12.00013 Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells. SHOU-CHENG ZHANG, Stanford University, B. ANDREI BERNEVIG, Princeton University, TAYLOR HUGHES, Stanford University — We show that the Quantum Spin Hall Effect, a state of matter with topological properties distinct from conventional insulators, can be realized in HgTe/CdTe semiconductor quantum wells. By varying the thickness of the quantum well, the electronic state changes from a normal to an “inverted” state at a critical thickness $d_c$. We show that this transition is a topological quantum phase transition between a conventional insulating phase and a phase exhibiting the QSH effect with a single pair of helical edge states. We also discuss the methods for experimental detection of the QSH effect.

Monday, March 5, 2007 8:00AM - 10:48AM — Session A13 DMP GMAG: Focus Session: Multiferroics I Colorado Convention Center Korbel 4C

8:00AM A13.00001 Magnetic Symmetry of Two-Dimensional Multiferroics. AVADH SAXENA, TURAB LOOKMAN, Los Alamos National Lab — Hexagonal rare earth manganites are multiferroic materials which exhibit triangular antiferromagnetic ordering in the basal plane which can be characterized by two-dimensional (2D) magnetic symmetry. Reduced dimensionality is also desirable for achieving large (usually nonlinear) magnetoelectric coupling at higher temperatures. Indeed, the magnetization in BaMnF$_2$ orders two dimensionally below the transition temperature with a change in the b-axis dielectric constant. Moreover, there can be phase transitions between different 2D magnetic phases. From this perspective we study two dimensional magnetic (or color) symmetry, enumerate 2D magnetic space groups and illustrate their role in multiferroic phase transitions.

8:12AM A13.00002 Rotation of orbital stripes and the consequent charge-polarized state in Pr(Sr,Ca)$_2$Mn$_2$O$_7$. YUSUKE TOKUNAGA, THOMAS LOTTERMOSER, YUANSANG LEE, ERAITO-JST, REIJI KUMAI, CERC-AIST, MASAYA UCHIDA, ERAITO-JST, TAKAHISA ARIMA, ERAITO-JST, Tohoku Univ., YOSHINORI TOKURA, ERAITO-JST, The Univ. of Tokyo — Nano-scale self-organization of electrons is ubiquitously observed in correlated-electron systems such as complex oxides of transition metals. The phenomenon of charge ordering (CO) or the formation of charge stripes, as observed for layered-structure cuprates and nickelsates, is one such example. Among them, the CO in the manganites is closely tied to the orbital degree of freedom of 3d electrons, leading to the staggered orbital ordering (OO) or the formation of orbital stripes in the layered structure. Here, we present the phenomena of thermally-induced rotation of the orbital stripes by 90 degrees for bilayered manganese Pr(Sr$_{1-2x}$Ca$_x$)$_2$Mn$_2$O$_7$(x=0.9) with half hole-doping, i.e., a 1:1 ratio of Mn$^{3+}$/Mn$^{4+}$ [1]. The rotation of orbital stripes and the consequent CO coupled with the underlying lattice distortion were found to produce the charge-polarized state, as also evidenced by its activity of optical second harmonic generation. [1] Y. Tokunaga et al., Nature Materials, doi:10.1038/nmat1773 (2006).

1This work was in part supported by Grant-in-Aids for Scientific Research from the MEXT, Japan.
Structural changes related to dielectric anomalies in RFeO$_4$ (R=Lu and Y).

Interaction, and I will discuss the possibility of electric-field induced magnetization switching in prototypical multiferroic systems such as BiFeO$_3$. These methods to understand the intriguing properties of presently known multiferroics and to design new multiferroic materials with more desirable properties.

Functional theory have made invaluable contributions to the present understanding of such magnetoelectric multiferroics. In this talk I will show how we use structural change due to the charge ordering in the three-dimensional hexagonal plane. We examined structural change by obtaining the electron diffraction (ED) patterns in the warming process and found that successive structural phase transition takes place around 220K. It is considered that these transitions should be characterized as the change of the charge ordering pattern in the hexagonal plane and are strongly correlated to the anomalous dielectric properties found in YFeO$_3$.

8:36AM A13.00004 X-ray Magnetic Circular Dichroism Investigation of Fe Valence Ordering in Multiferroic LuFeO$_4$. VEMURU KRISHNAMURTHY, Arkiv Ges National Laboratory, JONATHAN LANG, DANIEL HASSEL, GEORGE SRAJER, Argonne National Laboratory, BRIAN SALES, Oak Ridge National Laboratory, MAS SUBRAMANIAN, Oregon State University, DAVID SINGH, LEE ROBERTSON, MANUEL ANGST, DAVID MANDRUS, Oak Ridge National Laboratory. A new mechanism of ferroelectricity that is based on the iron valence ordering in a charge frustrated lattice has been reported for LuFeO$_4$. In this compound, a ferroelectric transition occurs at 330 K and ferromagnetic order develops below 250 K. The ferroelectric polarization shows a sharp increase at the ferrimagnetic ordering temperature suggesting that the two order parameters are coupled. X-ray magnetic circular dichroism (XMCD) at the Fe K edge and at Lu L$_2$L$_3$ edges has been measured in LuFeO$_4$ using 4-ID-D beamline at Advanced Photon Source. Two clear peaks are seen in the Fe K-edge XMCD suggesting that the magnetism of Fe is associated with two types of Fe sites. Fe K edge XMCD probes the 4p shell, thus it is sensitive to different charge states and gives an indirect measure of the Fe magnetism through 3d-4p hybridization. The observed double peak structure in the XMCD is an indication of charge ordering of Fe$^{2+}$ and Fe$^{3+}$ in the ferrimagnetic state. XMCD is also observed at Lu L$_2$L$_3$ edges suggesting a small induced Lu 5d moment. Funded by US Dept. of Energy.

8:48AM A13.00005 Spin-Charge-Orbital States and Electric Polarization in Multiferroic RFeO$_4$. SUMIO ISHIHARA, MAKOTO NAKA, JYUJI NASU, AYA NAGANO, Department of Physics, Tokohu University. Layered iron oxides RFeO$_4$ (R: rare-earth ion) is recognized to be an electronic ferroelectric and multiferroic compounds. Crystal structure of this compound is stacked of FeO$_2$ triangle layers. Charge and spin states have been studied by the electron and neutron diffraction experiments. Long range charge and spin orders characterized by the moment (1/3, 1/3) appear around 320K and 250K, respectively, in LuFeO$_4$. Electric polarization is induced around the charge ordering temperature of Fe$^{2+}$ and Fe$^{3+}$, and is enhanced around the magnetic ordering temperature. We examine theoretically spin-charge-orbital structures and electric polarization in RFeO$_4$. We suggest that Fe$^{3+}$ ion has the doubly degenerate orbital degree of freedom. Effective Hamiltonian for spin, charge and orbital degrees of freedom is derived. Numerical analyses with the multi-canonical Monte-Carlo simulation and the mean-field approximation show that the electric polarization is attributed to the charge order with momentum (1/3, 1/3). A magnitude of the polarization is enhanced around the magnetic ordering temperature due to the coupling between spin and charge. Conventional orbital order is not expected from the numerical calculation, and possible orbital states at low temperatures are discussed.

9:00AM A13.00006 Charge ordering and ferroelectricity in magnetite. DANIEL KHOMSKII, II. Physikalisches Institut, Universitat zu Koeln. Magnetite Fe$_3$O$_4$ is one of the most fascinating material in solid state physics. Besides being the first magnetic material known to the mankind, it is also the first example of an insulator-metal transition in transition metal oxides – the famous Verwey transition [1]. One usually connects this transition with the charge ordering of Fe$^{2+}$ and Fe$^{3+}$. However the detailed pattern of CO in Fe$_3$O$_4$ is still a matter of debate. Another aspect, which is not so widely known and which did not yet receive sufficient attention, is that below T$_V$, besides being completely spin polarised, magnetite apparently is also ferroelectric (FE) [2]. Thus it seems that magnetite, besides being the first magnetic material and the first transition metal oxide with an insulator-metal transition, is also the first multiferroic material. Using the idea of coexistence of site-centred and bond-centred charge ordering [3], I suggest a novel type of ordering in magnetite which explains the observed FE in Fe$_3$O$_4$ and which agrees with the structural data.


9:12AM A13.00007 Lattice and Magnetic Effects on Multiferroic Transitions in Garnets. DESPINA LOUCA, K. KAMAZAWA, U of Virginia. The combination of magnetic and ferroelectric properties in a single material is very appealing both because of the interesting coupling effects that emerge as well as due to a variety of technological applications that can be envisaged. Computational methods based on density functional theory have made invaluable contributions to the present understanding of such magnetoelectric multiferroics. In this talk I will show how we use these methods to understand the intriguing properties of presently known multiferroics and to design new multiferroic materials with more desirable properties. In particular, I will focus on the coupling between structural distortions and so-called "weak" magnetic order that is mediated by the Dzyaloshinskii-Moriya interaction, and I will discuss the possibility of electric-field induced magnetization switching in prototypical multiferroic systems such as BiFeO$_3$ and BaNiF$_2$. 

9:24AM A13.00008 Magnetoelectric coupling in multiferroic materials from first principles. CLAUDE EDERER, Columbia University. Magnetoelectric coupling in multiferroic materials is a very appealing both because of the interesting coupling effects that emerge as well as due to a variety of technological applications that can be envisaged. Computational methods based on density functional theory have made invaluable contributions to the present understanding of such magnetoelectric multiferroics. In this talk I will show how we use these methods to understand the intriguing properties of presently known multiferroics and to design new multiferroic materials with more desirable properties. In particular, I will focus on the coupling between structural distortions and so-called "weak" magnetic order that is mediated by the Dzyaloshinskii-Moriya interaction, and I will discuss the possibility of electric-field induced magnetization switching in prototypical multiferroic systems such as BiFeO$_3$ and BaNiF$_2$. 

9:30AM A13.00009 Structural evolution in the transition to the multiferroic state in SmFeO$_3$. T. LOUCA, K. KAMAZAWA, U of Virginia. The combination of magnetic and ferroelectric properties in a single material is very appealing both because of the interesting coupling effects that emerge as well as due to a variety of technological applications that can be envisaged. Computational methods based on density functional theory have made invaluable contributions to the present understanding of such magnetoelectric multiferroics. In this talk I will show how we use these methods to understand the intriguing properties of presently known multiferroics and to design new multiferroic materials with more desirable properties. In particular, I will focus on the coupling between structural distortions and so-called "weak" magnetic order that is mediated by the Dzyaloshinskii-Moriya interaction, and I will discuss the possibility of electric-field induced magnetization switching in prototypical multiferroic systems such as BiFeO$_3$ and BaNiF$_2$. 

9:36AM A13.00010 Multiferroic properties and phase transitions in some rare-earth iron garnets. A. L. LIMONOV, I. A. SAVICHEVA, I. A. PONOMAREV, M. V. DAVYDOV, V. A. EVSTIGNEEV, A. A. CHERNIKOV, Institute of Physics, RAS. Technological applications of magnetoelectric multiferroics are often based on the coupling between charge, orbital, and spin degrees of freedom. The finding of magnetoelectric multiferroics in single-iron garnet compounds sets the stage to explore the origin of electric polarization in these systems. In this work we find that the electric polarization in RFeO$_4$ compounds (R=Pr, Tb) originates from the spin-reorientation transition. The electric polarization is induced in these compounds below a characteristic temperature $T_{SO}$, which is higher than the magnetic ordering temperature. The electric polarization is induced in these compounds below a characteristic temperature $T_{SO}$, which is higher than the magnetic ordering temperature. We find that the electric polarization in these compounds is induced by the spin-reorientation transition. The electric polarization is induced in these compounds below a characteristic temperature $T_{SO}$, which is higher than the magnetic ordering temperature. We find that the electric polarization in these compounds is induced by the spin-reorientation transition. The electric polarization is induced in these compounds below a characteristic temperature $T_{SO}$, which is higher than the magnetic ordering temperature.
10:12 AM A13.00010 Systematic investigation of rare-earth doped BiFeO$_3$ thin films using composition spreads, S. FUJINO(1), V. NAGARAJAN(2), M. MURAKAMI(1), S.-H. LIM(1), A. VARTHARAJAN(2), L. SALAMANCA-RIBA(1), M. WUTTIG(1), I. TAKEUCHI(1)(3) — (1) Department of Materials Science and Engineering, University of Maryland, USA (2) University of New South Wales, AU (3) Center for Superconductivity Research, University of Maryland, We have systematically investigated compositionally varied rare-earth (RE) doped BiFeO$_3$ thin films using the combinatorial approach. Epitaxially grown (Bi$_{1-x}$RE$_x$)$_2$FeO$_4$ composition spread thin films were fabricated by laser molecular beam epitaxy on SrTiO$_3$ (001) substrates with an SrRuO$_3$ buffer layer. Transmission electron microscopy of the films showed that homogeneous epitaxial films were obtained throughout the composition range. Structural properties of (Bi$_{1-x}$RE$_x$)$_2$FeO$_4$ was mapped using scanning x-ray diffraction, and structural transitions were observed at various compositions. In some compositions, substantial enhancement in ferroelectric properties was observed at the structural transition: increase in the dielectric constant, increase in the piezoelectric response, and decrease in the coercive field were observed, while high polarization is maintained. Detailed dependence of various properties on composition variation will be discussed. Work supported by NSF DMR 0094265, DMR 0231291, MRSEC DMR-00-0520471 and the W. M. Keck Foundation.

10:24 AM A13.00011 Exchange bias between ferromagnetic metals and multiferroic BiFeO$_3$, LuMnO$_3$, and TbMnO$_3$, MAKOTO MURAKAMI, S. FUJINO, J. HATTRICK-SIMPERS, S.-H. LIM, L. SALAMANCA-RIBA, D. KUNDALIYA, S. OGALE, T. VENKATESAN, J. HIGGINS, M. WUTTIG, I. TAKEUCHI, University of Maryland, S. LOFLAND, Rowan University, S.-W. CHEONG, Rutgers University — We have used exchange bias at ferromagnet/layer/multiferroic interfaces to study the nature of magnetism in multiferroic materials. Co 5 nm layers have been deposited by sputtering on surfaces of epitaxial BiFeO$_3$ and TbMnO$_3$ thin films and on LuMnO$_3$ single crystals. Epitaxial BiFeO$_3$ and TbMnO$_3$ films were prepared by PLD. Magnetic properties of the Co/multiferroic bilayers are measured using SQUID, VSM, MOKE and XMCID. In BiFeO$_3$, we find that the bilayers exhibit exchange bias even at room temperature. In the TbMnO$_3$ system, increasing of coercive field and exchange bias was also clearly observed below the Néel temperature. In LuMnO$_3$, we observe positive exchange bias as well as switching of the sign of the exchange bias depending on the cooling procedure. This behavior may be related to the frustration in Mn spins. Difference in the exchange bias behavior between different multiferroic materials will be discussed. The effect of electric field on exchange bias is currently under investigation. Supported by ONR N000140110761, ONR N00014010085, NSF DMR 0094265, DMR 0231291, MRSEC DMR-00-0520471, and the W. M. Keck Foundation.

10:36 AM A13.00012 Charge ordering as alternative to Jahn-Teller distortion, IGOR MAZIN, Naval Research Laboratory, DANIEL HOMSKII, II Physikalisches Institut, Universitaet zu Koeln — It was pointed out in the seminal paper of Jahn and Teller that a partially occupied degenerate molecular level, often a doubly degenerate $E_g$ level in a cubic ligand field, is unstable against a distortion that splits the level and lowers the total energy of the occupied states. Since then, this effect has been commonly found in solids where it takes a form of a cooperative Jahn-Teller (JT) effect (orbital ordering), when the crystal lattice distortion coherently so as to lift orbital degeneracy at each site or, in band language, to split an entire band ($e_g$, $e_u$) and thus open a gap at the Fermi level. Upon the gradual delocalization of degenerate electrons, the JT distortion and corresponding orbital ordering becomes less and less favorable, but, as we show, below a crossover region exists with the possibility of lifting degeneracy not by an orbital ordering, but by a charge ordering (CO): an electron can be transferred from one ion to another, so that, say, the doubly degenerate $e_g$ level on one site will be fully occupied, and on the other site empty. In this paper we demonstrate, experimentally and by first principles calculations, that just such a “JTCO” effect actually occurs in the rare earth nickelates such as VNiO$_3$ and LuNiO$_3$. Apparently this novel phenomenon can also take place in other similar systems.

Monday, March 5, 2007 8:00 AM - 10:48 AM — Session A14 GMAG DMP FIAP: Focus Session: Spin Dependent Tunneling I Colorado Convention Center Korbel 4D

8:00 AM A14.00001 Spectroscopic Studies on epitaxially grown Fe/MgO/Fe magnetic tunnel junctions on W(100), TAE-YOUNG KHIM, JUN-SIK LEE, KEE-JEONG RHO, HOYOUNG JANG, BYEONG-GYU PARK, JAE-HOON PARK1, Dept. of Physics, POSTECH, Korea, JAE-YOUNG KIM, HANGIL LEE2, Beamline Research Division, PAL, Korea — In these days, there is a big interest in epitaxial Fe/MgO/Fe MTJ systems in the TMR issues. We investigated electronic states and magnetic behaviors of epitaxially grown Fe/MgO/Fe on W(100) at different MgO thicknesses using XAS, MCD, XPS, SRPES, and discussed a few noticeable phenomena in this system. First, XAS and MCD spectra at Fe $L_{2,3}$-, O K-, and Mg K$L_3$-$L_3$-edges varies as a function of MgO thickness. Second, in MgO/Fe/W(100), the magnetic hysteresis curve suddenly changes at a certain MgO layer thickness, probably due to a developed strain at the MgO/Fe interface. Finally, in Fe/MgO/Fe/W(100), an antiferromagnetic and a ferromagnetic interlayer coupling between two Fe ferromagnetic layers were observed for different MgO layer thicknesses, and we determined the spin polarization of the density of states.

1corresponding author
2corresponding author

8:12 AM A14.00002 Electronic structure of sputter deposited MgO(100) tunnel barriers in magnetic tunnel junction structures exhibiting giant tunneling magnetoresistance, SEE-HUN YANG, IBM Almaden Research Center, MAHESH SAMANT, IBM Almaden Research Center, STUART PARKIN, IBM Almaden Research Center, IBM ALMADEN RESEARCH CENTER TEAM — Giant tunneling magnetoresistance (TMR) in magnetic tunnel junctions formed with crystalline MgO tunnel barriers [1] have potential applications in a wide variety of spintronic devices. However, the relationship of the TMR to the detailed chemical and electronic structure of the MgO barrier and its interfaces with the ferromagnetic electrodes is not yet fully understood. We have carried out valence band photoemission spectroscopy and x-ray absorption spectroscopy to characterize the chemical state and electronic structure of sputter deposited, highly oriented, MgO (001) barriers and its interfaces with ferromagnetic electrodes. A large band gap of ~7.5 eV is found even for ultrathin MgO layers. This is consistent with barrier heights found from fitting current versus voltage curves providing that very small effective electron masses are used. We discuss the role of thin Mg interface layers that we have used to reduce oxidation of the underlying ferromagnetic layer during the MgO layer formation [1]. [1] S. P. Parkin, C. Kaiser, A. Panchula, P. M. Rice, B. Hughes, M. Samant, S.-H. Yang, Nature Materials 3, 862 (2004).
PHUONG MAVROPOULOS, STEFAN BLUGEL — We determine from first principles the Curie temperature of bulk Co in the ground state hcp phase and the bcc-Co and its relation to Co/MgO/Co magnetic tunnel junctions, MARJANA LEZAIC, IFF, Research Center Juelich, PHIVOS MAVROPOULOS, STEFAN BLUGEL — We determine from first principles the Curie temperature of bulk Co in the ground state hcp phase and the bcc-Co and its relation to Co/MgO/Co magnetic tunnel junctions.

Is found to quench the TMR but less strongly than roughness. Channel. Roughness is found to quench these resonances leading to a drastic reduction of TMR to values comparable to those seen in experiment. Leads disorder is included in the transport calculation using large lateral supercells. In our study we found that in case of ideal, perfectly ordered systems, the values of TMR comparable in size to those predicted by others in which the mechanism responsible is the very effective transmission through resonant states close to the Fermi level for the minority spin.

In observing large values of tunnelling magnetoresistance (TMR) in epitaxial FeCo/MgO/FeCo magnetic tunnel junctions (MTJ’s), the values reported are still two orders of magnitude lower than those predicted by first-principles transport calculations for ideal, defect-free MTJ’s. In this talk, we present results of a systematic study of the influence of roughness and leads disorder on TMR in a FeCo/vacuum/FeCo model system. Our study is based upon a tight-binding muffin-tin orbital (TB-MTO) implementation of the Landauer-Büttiker scattering theoretical formulation of transport. Disorder is included in the transport calculation using large lateral supercells. In our study we found that in case of ideal, perfectly ordered systems, the values of TMR comparable in size to those predicted by others in which the mechanism responsible is the very effective transmission through resonant states close to the Fermi level for the minority spin channel. Roughness is found to quench these resonances leading to a drastic reduction of TMR to values comparable to those seen in experiment. Leads disorder is found to quench the TMR but less strongly than roughness.

8:36AM A14.00044 First-principles prediction of high Curie temperature for ferromagnetic bcc-Co and its relation to Co/MgO/Co magnetic tunnel junctions. MARJANA LEZAIC, IFF, Research Center Juelich, PHIVOS MAVROPOULOS, STEFAN BLUGEL — We determine from first principles the Curie temperature of bulk Co in the ground state hcp phase and the metastable fcc and bcc phases. For fcc-Co we found a Curie temperature of \( T_C^{\text{fcc-Co}} = 1280 \, \text{K} \), in reasonable agreement with experimental results. For bcc-Co, a Curie temperature of \( T_C^{\text{bcc-Co}} = 1400 \, \text{K} \) is predicted. This suggests that bcc-Co/MgO/bcc-Co tunnel junctions offer high tunneling magnetoresistance ratios even at elevated temperatures, giving them an advantage over Fe/MgO/Fe junctions. \( T_C^{\text{bcc-Co}} \) appears robust under tetragonalization upon epitaxial growth on MgO, in contrast to Fe for which \( T_C^{\text{bcc-Fe}} \) is found to drop by more than 20% (from 970 K to 750 K) upon such a tetragonalization. We find that FeCo alloys have an even higher \( T_C \), as high as 1660 K for ordered FeCo. We discuss the origin of these effects in terms of the electronic structure and densities of states. The Curie temperatures are calculated by mapping ab initio results to a Heisenberg model, which is solved by a Monte Carlo method.

8:48AM A14.00005 Theory of the spin-orbit induced anisotropy in the tunneling magnetoresistance of magnetic tunnel junctions.1 ALEX MATOS-ABIAGUE, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — We investigate the effects of the spin-orbit interaction on the tunneling magnetoresistance of magnetic tunnel junctions. We propose a theoretical model in which the two-fold symmetry of the tunneling anisotropic magnetoresistance (TAMR) effect, observed in Fe/GaAs/Au tunnel junctions, originates from the interference between Dresselhaus and Bychkov-Rashba spin-orbit couplings at the interface between the ferromagnetic (Fe) region and the GaAs tunnel barrier. Bias induced changes of the Bychkov-Rashba spin-orbit coupling can result in a flipping of the axis of the two-fold symmetry of the TAMR. The theoretical results are in good agreement with recent experiments [1].

Financial support by German Science Foundation (DFG) via SFB 689 is gratefully acknowledged.

9:00AM A14.00006 Bias induced inversion of the tunneling magnetoresistance. ANDREJ SOKOLOV, University of Nebraska-Lincoln, RENAT SABIRIANOV, University of Nebraska-Omaha, ILDAR SABIRIANOV, University of Nebraska-Lincoln, BERNARD DOUDIN, IPCMS, Strasbourg — Demand for high density at low cost two-terminal nonvolatile memory devices has boosted research interest in electroreversible phenomena where conductivity exhibits voltage-induced resistance jump up to several orders in magnitude. NiO based junctions are particularly promising because of its high ON/OFF ratio and simple constituents. We report low temperature transport properties of electrochemically synthesized Ni/NiO/Co/NiO/Co magnetic double barrier tunneling junction (MTJ) in nanowires with diameter of 70nm, and NiO barrier thickness of about 2 nm. Resistance bistability of double NiO nanojunctions is observed and reaches 100%. We observe the sign inversion of the tunnel magnetoresistance upon resistance switching from low-resistance (LR) to high-resistance (HR) state, indicating a new resonant tunneling path promoted by an applied voltage bias. Thus our MTJ shows multifunctional properties with four resistance states which can be manipulated by applied electric and magnetic fields. This device can be used as a four-state logic gate or memory cell with multifunctional properties. The interpretation in terms of occupation-driven metal-insulator transition in one of the two junctions is proposed, explaining switching of the resistance and the magnetoresistance.

9:12AM A14.00007 Evidence for WKB Failure in Contemporary Magnetic Tunnel Junctions.1 CASEY W. MILLER, University of California, San Diego — This work describes evidence for the failure of the WKB approximation in state-of-the-art magnetic tunnel junctions. Surprisingly, the tunneling conductance of three varieties of CoFeB/MgO/CoFeB magnetic tunnel junctions depends quadratically on the applied voltage to anomalously high biases: the parabolic conductance persists to 2 V, greater than half the theoretical MgO barrier height. Within the framework of WKB, these data imply unphysical barrier parameters. We show that the origin of this breakdown is a distribution of barrier thicknesses consistent with experimentsally inferred interface roughness, possibly in conjunction with the tunneling electron sensing the MgO band structure. Additionally, well defined and reproducible bias-dependent conductance oscillations are observed in CoFeB/MgO/NiFe devices. These oscillations are mediated by the reflection of tunneling electrons from the sharp MgO/NiFe interface, which allows electron standing waves to form within the MgO barrier. The oscillation amplitude is enhanced in the antiparallel state, which gives rise to oscillations of the tunneling magnetoresistance. A model employing spin-split free electron bands and the exact solution to the Schrödinger equation demonstrates qualitative agreement with the data. This work implies that using existing WKB-based models may lead to physically incorrect barrier parameters for contemporary tunnel junctions, which may underscore the imminent necessity for first principles analyses of contemporary tunneling devices with textured or epitaxial barriers, MgO or otherwise.

1 In collaboration with Z.-P. Li, I. K. Schuller, R. W. Dave, J. Slaughter, and J. Akerman. Supported by US-DOE.

9:48AM A14.00008 Highly charged ion modified magnetic structures. HOLGER GRUBE, JOSHUA POMEROY, National Institute of Standards and Technology, ANDREW PERRELLA — Highly charged ions (HCIs) deposit large amounts of energy very locally in small areas of only a few square nanometers per HCI impact. This allows for the modification of nanometer sized areas and the creation of nanosized features on impact surfaces. We have used highly charged ions such as Xe\(^{4+}\) to modify ultrathin oxide barriers in magnetic tunnel junctions (MTJs) in order to locally change their electrical properties. We have been able to drastically reduce the resistance area (RA) product of our Co/Al-Ox/Co MTJs. While the magnetoresistance of HCI modified MTJ is also reduced, we created a new hybrid magnetic field sensor composed of tunnel and metallic junctions. We have analyzed the properties of individual HCI created conduction channels through ensemble measurements. Generalizing this approach, HCIs can be used to create hybrid materials through the introduction of nanometer sized electric or magnetic channels. This could be a useful tool to probe materials properties and physics on the nanometer scale.

1Support provided by the US-DOE through the National Institute of Standards and Technology (NIST).
10:00AM A14.00009 Tunneling anisotropic magnetoresistance in Ni break junctions, J. D. BURTON, E. Y. TSYMBAK, University of Nebraska Lincoln, O. N. MRYASOV, Seagate Research — Anisotropic magnetoresistance (AMR) is the difference in resistance as the magnetization direction is changed with respect to the direction of current flow. We will present results of first-principles calculations of AMR in Ni nanowires. It is known that in the ballistic regime the conductance of a magnetic nanowire changes in steps of $e^2/h$ as the angle of the magnetization changes with respect to the axis of the wire.[1] This ballistic AMR (BAMR) effect originates from the spin-orbit coupling which can change the number of bands crossing the Fermi energy ($E_F$) as the magnetization direction is changed. We extend this consideration to the case of a break junction, where transport occurs via tunneling. We find a significant dependence of the tunneling conductance on the magnetization direction, an effect known as tunneling AMR (TAMR). We find that states localized at the electrode tips near the break are broadened by the spin-orbit interaction and contribute significantly to the tunneling. The position with respect to $E_F$ and broadening of these states depend strongly on the orientation of magnetization. Our results bear a striking resemblance to recent experimental results[2], clearly indicating an origin different from the one proposed previously.[2] This work is supported by Seagate Research and Nebraska NSF-MRSEC. [1] J. Velev et al. PRL 94, 127203 (2005), [2] K. Bolotin et al. PRL 97, 127202 (2006).

10:12AM A14.00010 Magnetoresistance in Boron Carbide junctions, ELENNA DAY, A. SOKOLOV, A. BARUTH, B.W. ROBERTSON, S. ADENWALLA, University of Nebraska-Lincoln — The properties of thin insulator layers are crucial to the performance of magnetic tunnel junctions. Commercial requirements are a device with a high tunnel magnetoresistance (TMR) with low cost and high stability. At present the vast majority of barriers are made from amorphous Al$_2$O$_3$ and crystalline MgO. The TMR value depends not only on the spin-dependent electronic structure of the electrodes, but on the metal-insulator interface. Oxide-type barriers may suffer from local vacancies and other type of defects, resulting in oxygen diffusion, making the TMR value unstable with time. We present TMR results obtained on a nonoxide barrier, boron carbide (B$_{10}$C$_2$) for applications in magnetic tunnel junctions. This low Zorganic material can be grown by plasma enhanced chemical vapor deposition (PECVD) without pinholes in the ultra thin film regime. PECVD grown boron carbide is an excellent dielectric with resistivities in the range of 10$^9$ ohm-cm, with a band gap that can be adjusted from 0.7 eV to 1.9 eV by altering the boron to carbon ratio and to band gap values well above 2.7 eV by adding phosphorus. This creates a unique opportunity for experimental study of a broad spectrum of phenomena, related to the dielectric properties of the barrier.

1 Supported by the NSF through the MRSEC, DMR and CHE depts.

10:24AM A14.00011 Inelastic Electron Tunneling Spectroscopy of a Molecular Magnetic Tunnel Junction, WENYONG WANG, CURT RICHTER, National Institute of Standards and Technology — We present the results of systematic measurements of molecular magnetic tunnel junctions (MTJs). In this study, we fabricated molecular-monolayer based MTJs and show that inelastic electron tunneling spectroscopy (IETS) can be utilized to characterize such junctions to investigate the existence of desired molecular species in the device area and to study the reported bias-dependence of junction tunneling magnetoresistance (TMR). Temperature-dependent current-voltage characteristics have been performed on the fabricated molecular MTJ with octanethiol as the molecular tunnel barrier. Tunneling transport has been observed at $T < 50K$. IETS measurement at $T = 4.2 K$ revealed spectra signatures due to $\nu(Ni-S)$, $\nu(C-S)$, and $\delta(CH_2)$ vibrational modes, thus confirming the presence of the molecular species confined inside the ferromagnetic-octanethiol molecular tunnel junctions. TMR measurements have been carried out and spin-dependent tunneling transport has been observed. A bias-dependence of the tunneling resistance has been observed. IETS measurements at different magnetic field suggest that the like cause of the TMR bias-dependence is inelastic scattering due to molecular vibrations.

10:36AM A14.00012 Towards Fully Organic Tunnel Junctions, BRIDGER ANDERSON, TONY CARUSO, MUNIR KADERBHAI, CNSE — Quantum mechanical tunneling through ultrathin (25 A) insulating materials has been experimentally verified since the 1950’s. Recently, it has become possible to fabricate organic based materials and single molecules occurred from inorganic metallic injectors. We present here our effort focused on fabrication and characterization of an organic tunnel junction where the injector is a conducting polymer and discuss the subtle difference which stem from polaronic metal.

Monday, March 5, 2007 8:00AM - 10:48AM
Session A18 DPOLY DMP: Photophysics of Electronic Polymers Colorado Convention Center 103

8:00AM A18.00001 Identification of the Possible Defect States in Poly(3-hexylthiophene) Thin Films, DANQIN FENG, University of Nebraska-Lincoln, ANTHONY CARUSO, North Dakota State University, YAROSLAV LOSOVYJ, Louisiana State University, DOUGLAS SCHULZ, North Dakota State University, PETER DOWBEN, University of Nebraska-Lincoln — We find evidence for a gradual change in the electronic properties of regioregular poly(3-hexylthiophene) thin films with temperature. The conduction properties appears to be mediated by hopping conduction dominated by a low density of defects states within the highest occupied molecular orbital to lowest unoccupied molecular orbital gap, not by a change in band gap. The possible origins of a low density of defects states within the highest occupied molecular orbital to lowest unoccupied molecular orbital gap are suggested. A number of “chemical” defects, impurities and structural defects can contribute to features in photoemission for regioregular poly(3-hexylthiophene). A density of states within the highest occupied molecular orbital to lowest unoccupied molecular orbital gap may affect the transport properties of regioregular poly(3-hexylythiophene) and like polymers. These gap electronic states are not expected in the perfectly ordered polymer.

8:12AM A18.00002 Ab initio study of ladder-type metallic polymers, SIMON PESANT, GUILLAUME DUMONT, SEBASTIEN LANDGEVIN, MICHEL COTE, Departement de physique, Universite de Montreal — The electronic structure of recently synthesized ladder-type polythiophene polymer is studied with density-functional theory based calculations. It is found, in the local density approximation (LDA) that when a simple substitution of the sulfur atoms by nitrogen and boron atoms, the band structure of the resulting polymer (called LPPyB) exhibits bands overlap between the occupied and the unoccupied states that is characteristic of metallic systems. The band structure is further validated by GW calculations confirming the assessment of the LDA results. Calculations using the B3LYP functional, which contains exact exchange, show a different electronic behavior, a small HOMO-LUMO band gap of 0.67 eV is obtained. In order to better assess the energy gap of the polymer, a TDDFT (Time-dependent density-functional theory) study of the LPPyB was performed on oligomers and verifies the metallic structure of this polymer. Other calculations were done using TDDFT on different polymers to validate the last result. In parallel, similar electronic properties were computed on an isoelectronic polymer of LPPyB, having the atomic structure of the ladder- type polythiophene, with only one sulfur atom replaced by a boron atom.

8:24AM A18.00003 Illumination induced metastable polaron-supporting phase in poly-p-phenylene- vinylen films, E. EHRENREUD, E. GERSHAM, Y. EICHEN, Technion-Israel Institute of Technology, T. DRORI, C.X. HENG, Z.Y. VARDENY, University of Utah — We found a new illumination induced metastable polaron-supporting phase in pristine films of a soluble derivative of poly-p-phenylene vinylene (MEH-PPV). In the pristine, un-illuminated MEH-PPV phase A, the polymer films do not show any long-lived photogenerated polarons. Prolonged UV illumination, however, was found to induce a reversible, metastable phase B, characterized by its ability to support the existence of abundant long-lived photogenenated polarons. In the dark, films of phase B revert back to the original phase A within about thirty minutes at room temperature. Relying on the well-established ubiquitous reversible photoinduced cyclization of diarylethenes into dihydrophenanthrene derivatives, we propose a reversible mechanism in which UV illumination creates metastable deep defects that substantially increase the photogenenated polaron lifetime.
8:36AM A18.00004 Ultrafast and Nonlinear Optical Spectroscopies of Excited States in Pristine and Doped π-Conjugated polymers1, VALY VARDENY, University of Utah — A variety of ultrafast and optical nonlinear spectroscopies were applied to pristine and doped π-conjugated polymers, for elucidating the excited states energy levels and primary photoexcitation species in these materials. These spectroscopies include fs pump-probe photomodulation (PM), two-photon absorption (TPA), photoluminescence up-conversion (PL(t)), and electroabsorption (EA); as well as THz time domain spectroscopy (THz-TDS). The π-conjugated polymers include derivatives of PFO, PPV and PT, as well as t-(CH)x; doping includes fullerene molecules, as well as heavily doping with strong acceptors. The results have been analyzed in terms of the exciton picture advanced by Mazumdar et al. The primary photoexcitations are singlet excitons of which PM spectrum is composed of two strong photoinduced absorption bands in the mid and near ir spectral range, that are correlated with a stimulated emission band and PL(t). These bands are in agreements with transitions from the lowest exciton with odd symmetry into higher lying excitons with even symmetry, as revealed by TPA and EA spectroscopies. Polaron excitations are also formed and are characterized by two bands in the mid-ir range, and correlated ir-active vibrations. Surprisingly t-(CH)x is different from many other π-conjugated polymers, except that the primary polarons recombine at a later time to form charged solitons. In fullerene-doped polymers the primary singlet excitons are trapped and undergo ultrafast nonradiative decay in doping-related defects, and this explains in part the weak cw PL in these compounds. In heavily doped polymers with strong acceptors the ground state no longer is neutral, but rather contains substantial amount of free charge carriers characterized by the Drude free carrier response in the THz to mid ir spectral ranges.

1Supported in part by the DOE grant 04ER46109, and the NSF DMR 05-03172

9:12AM A18.00005 Temperature dependence and anisotropy of charge-carrier mobilities in crystalline durene , FRANK ORTMANN, KARSTEN HANNEWALD, FRIEDHELM BECHSTEDT, Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitaet, Max-Wien-Platz 1, 07743 Jena, Germany — We report on the theoretical analysis of charge-carrier mobilities in durene crystals. The crystal is studied with DFT methods to examine structural, vibrational, and electronic properties. On that basis we employ a Holstein-Peierls model (see Hannewald et al. PRB 69, 075211 (2004); PRB 69, 075212 (2004)) to simulate the temperature dependence of the mobilities. The relation between the anisotropy of electron/hole mobilities and the band structure as well as lattice vibrations is discussed.

9:24AM A18.00006 Ultrafast polarization memory dynamics of photoexcitations in π-conjugated polymers., SANJEEV SINGH, MINGHONG TONG, JOSH HOLT, ZEEV VARDENY, Physics Department, University of Utah — For better understanding ultrafast photoexcitation dynamics in π-conjugated polymers, we study the polarization memory dynamics in the pump/probe photomodulation (PM) spectrum of these materials. The transient PM spectrum of polymers contain singlet excitons with prominent photoinduced absorption (PA) band, stimulated emission and photobleaching bands in the near ir/visible spectral range; polarons with PA bands in the mid- and near-ir; and polaron pairs in the visible range. Each of these spectral feature shows polarization memory, P(t) where the PM signal with parallel pump/probe polarizations is ~ twice larger with than perpendicular polarizations. P(t) has a specific dynamics for each photoexcited species, and, in addition it also depends on the excitation pump photon energy. Results for MEH-PPV films and solutions will be thoroughly discussed, in comparison with the photoluminescence efficiency.

9:36AM A18.00007 Experimental Determination of Charge/Neutral Branching Ratio in π-Conjugated Polymers by Broad-band Ultrafast Spectroscopy1, CHUANXIANG SHENG, MINGHONG TONG, SANJEEV SINGH, Z. VALY VARDENY, Physics Department, University of Utah, Salt Lake City, Utah 84112, USA — We demonstrate a reliable method of determining the branching ratio, η of photogenerated charge (polarons) to neutral (excitons) photoexcitations in various π-conjugated polymer films and solutions using femtosecond ultrafast spectroscopy with broad spectral range from 0.14 to 2.7 eV. We found that both excitons and polarons are instantaneously photogenerated, but η critically depends on the film nanomorphology, which, in turn controls the interchain coupling. In films, η varies between 1% for derivatives of poly(p-phenylene vinylene) casted from chloroform solution, to more than 30% for regio-regular poly-3-hexyl thiophene. Our results show that charge photogeneration quantum efficiency in these materials is an interchain process; and this has ramifications for their use in solar cell applications. 1Supported in part by the DOE.

9:48AM A18.00008 In-situ characterization of the mesophase of a high performance semiconductor, L.J. RICHTER, A.J. MOAD, D.M. DELONGCHAMP, R.J. KLINE, D.J. GUNDLACH, D.A. FISCHER, NIST, Gaithersburg, MD — Poly(2,5-bis(3-alkyliothiophen-2-yl)thieno[3,2-b]thiophene) is a semiconducting polymer with exceptional hole mobility in thin film transistors upon annealing into a mesophase. We have identified the structural motifs of both the mesophase and the high performance, thermally processed film with a variety of in-situ techniques: NEXAFS, spectroscopic ellipsometry (SE), and IR absorption. Upon cooling from the mesophase, the films exhibit π-stacked lamella with molecular terraces (AFM) with a high degree of order of the concatenated backbone (NEXAFS). The side chains are well ordered (IR) and interdigitated, which may be a driving factor in the growth of large crystals. Upon re-heating, the side chains (IR) and conjugation length (SE) monotonically disorder until entry into the mesophase which is characterized by highly disordered side chains and moderate torsional disorder of the backbone but near ideal in-plane order of the polymer long axis. Side-chain order is reestablished upon re-cooling into the ordered phase. The hysteresis of the side chain order mimics the DSC of powders. As-cast films exhibit greater disorder in all degrees of freedom; entry into the mesophase is necessary to achieve high order. The spectroscopic data can be correlated with in-situ mobility measurements.

10:00AM A18.00009 Electro-optic measurements in Single-Crystal Films of a Combination of Materials Involving DAST and IR-125 , A. NARAYANAN, J. TITUS, M. THAKUR, PHOTONIC MATERIALS RESEARCH LABORATORY, AUBURN UNIVERSITY, AL, 36849 TEAM — Single crystal films of a combination of materials involving DAST and a dye molecule IR-125 have been prepared using the modified shear method. X-ray diffraction results indicate a 001 orientation of the film similar to a DAST single-crystal film. The electro-optic measurements of the DAST-IR-125 films have been performed using field induced birefringence in the cross polarized geometry at 633 nm and 1550 nm. A modulation of 14 percent has been observed in a single pass through the film for a field of 1 Volt/micron at 633 nm. The results indicate exceptionally high electro-optic coefficients at both of the wavelengths (633 and 1550 nm).

10:12AM A18.00010 Nonlinear Refractive Index in a Novel Nano-optical Material Based on the Nonconjugated Conductive Polymer, Poly(β-pinene) , A. NARAYANAN, J. TITUS, MRINAL THAKUR — Two photon absorption in a novel nano-optical polymer based on the nonconjugated conductive polymer, iodine-doped poly(β-pinene) has been recently reported. In the present report, we will discuss measurement of the nonlinear refractive index (n2) of iodine-doped poly(β-pinene). The measurement has been made using 150 fs pulses from a Ti:Sapphire laser. Time-resolved measurement has been made using pump-probe technique in which the phase change in the probe beam was measured from the intensity-induced birefringence while the pump pulse was overlapped. The measured value of the nonlinear refractive index is larger than 10⁻⁹ cm²/W at 800 nm. The results show that the measured n2 is of electronic origin. This exceptionally large magnitude of n2 has been attributed to the special electronic structure of doped poly(β-pinene) confined in a sub-nanometer domain.
10:24AM A18.00011 Quadrupolar dyes for NLO applications: solvent-induced symmetry breaking and huge TPA cross-sections in aggregates , ANNA PAINELLI, GABRIELE D’AVINO, FRANCESCA TERENZIANI, Parma University — Quadrupolar dyes, where electron donor (D) and acceptor (A) groups are linked by π-conjugated bridges to yield symmetrical structures (D-π-A-π-D or A-π-D-π-A) are intensively studied for TPA applications. In an essential-state model for the solvated dyes, symmetry-broken dipolar solutions are found for either the ground or the one-photon excited state. Dyes are accordingly classified in three different classes, with distinctively different spectroscopic behavior. The model provides useful guidelines for the design of molecules for TPA applications and represents a general frame to understand energy transfer processes in multipolar molecular systems. [1] The same essential state model applies to aggregates of quadrupolar dyes. Relaxing the dipolar approximation for electrostatic intermolecular interactions, bound-biexcitons appear with important spectroscopic consequences. Specifically, the large TPA cross-section of quadrupolar dyes is amplified by orders of magnitude as a result of aggregation. [2] F. Terenziani, A. Painelli, C. Katan, M. Charlton, M. Blanchard-Desce, J. Am. Chem. Soc. 2006.

10:36AM A18.00012 Infrared probe of charge dynamics in single crystal rubrene organic field-effect transistors , ZHIQIANG LI, University of California, San Diego, VITALY PODZOROV, Rutgers University, NA SAI, University of California, San Diego, MICHAEL MARTIN, Lawrence Berkeley National Laboratory, MICHAEL GERSHENSON, Rutgers University, MASSIMILIANO DI VENTRA, DIMITRI BASOV, University of California, San Diego, UNIVERSITY OF CALIFORNIA, SAN DIEGO COLLABORATION, RUTGERS UNIVERSITY COLLABORATION, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION — We report on infrared (IR) spectroscopy of charge dynamics in organic field-effect transistors based on single crystal rubrene. IR microscopy measurements show uniform charge injection over macroscopic length scales of several millimeters in these devices. IR measurements uncover anisotropic optical conductivities of these transistors in agreement with earlier transport studies. The field-induced electronic excitations in rubrene reveal optical constants with the Drude-like form and low effective masses. I will discuss several new aspects of the charge dynamics in organic molecular crystals uncovered by this work.

Monday, March 5, 2007 8:00AM - 10:48AM —
Session A23 DMP DCOMP: Focus Session: High Pressure I - Earth and Planetary Materials Colorado Convention Center 110

8:00AM A23.00001 Characterization of Jupiter’s Interior with First Principles Computer Simulations , BURKHARD MILITZER, JAN VORBERGER, Carnegie Institution of Washington, WILLIAM HUBBARD, University of Arizona — We report results from recent investigations of the interior structures of Jupiter using density-functional molecular dynamics (DFT) simulations of dense fluid hydrogen-helium mixtures [1]. The equation of state (EOS) is derived on a grid of temperature and density points spanning Jupiter’s interiors. The properties of both fluids in dynamic shock compression experiments are compared [2]. Based on the DFT-EOS, we derive models for the interior of giant planets. Our models update the suite of models that were based on the widely used Saumon-Chabrier-Van Horn (SCVH) EOS. Unlike SCVH, the computed DFT-EOS does not predict any first-order thermodynamic discontinuities associated with pressure-dissociation and metatization of hydrogen. Deviations of the DFT-EOS from SCVH are up to about +/- 5% depending on the pressure. As a result our models predict a significantly larger rocky core for Jupiter than SCVH. We will discuss inferred core mass and make predictions for properties of core. [1] J. Vorberger, I. Tamblyn, B. Militzer, S.A. Bonev, “Hydrogen-Helium Mixtures in the Interiors of Giant Planets,” cond-mat/0609476. [2] B. Militzer, PRL 97 (2006) 175501. Supported by NASA PGG04-0000-0116 and NSF Grant 0507321.

8:12AM A23.00002 High pressure bonding properties of hydrogen1, ISAAC TAMBLYN, Dalhousie University, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, STANIMIR BONEV, Dalhousie University — There has been considerable experimental and theoretical effort to describe the transition in hydrogen from a molecular to non-molecular fluid. Resolution of discrepancies that continue to exist between different investigations of hydrogen is expected to have significant implications in fields such as planetary science. We have preformed three sets of first-principles simulations, constant density, pressure, and temperature, in order to study the molecular, non-molecular, and transition regimes of the hydrogen (deuterium) phase diagram. Constrained and unconstrained bond length simulations were used to examine changes that occur in the inter-atomic potential upon disassociation. By forcing the destruction of molecules in the molecular regime, and by considering the catalyzing effect of single hydrogen atoms, we have probed the mechanisms that drive this transition. Finally, spatial distributions of species surrounding molecules at the time of dissociation have provided insight into the structure of the liquid.

1Work supported by the NSERC of Canada. E.S. worked under the auspices of the U.S. Dept. of Energy at the University of California/LLNl under contract No. W-7405-Eng-48

8:24AM A23.00003 Computational study of the Hydrogen equation of state using the Coupled Electron-Ion Monte Carlo method , MIGUEL MORALES, Department of Physics, University of Illinois at Urbana-Champaign, KRIS DELANEY, Materials Research Laboratory, UCSB, DAVID CEPERLEY, Department of Physics, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, Dipartimento di Fisica, Universita del l’Aquila, l’Aquila, Italy — We study the equation of state of liquid Hydrogen at Mbar pressures, in the regime of pressure dissociation/ionization, using the Coupled Electron-Ion Monte Carlo (CEIMC) method. Our aim is to accurately describe the crossover from the molecular to the atomic regime. The CEIMC method is based on the Born-Oppenheimer approximation and consists of a Monte Carlo simulation of the ionic degrees of freedom (either with path integrals or classical Metropolis) using a potential energy surface obtained from a zero temperature QMC method. The electronic calculation is done using either Variational Monte Carlo or the more accurate Reptation Quantum Monte Carlo. A Slater-Jastrow wavefunction is used, with an analytical RPA Jastrow term and one-body orbitals obtained from a fast band structure calculation. Recently, we incorporated backflow corrections to the orbitals obtained from DFT. This results in a much improved wavefunction over the entire crossover regime. We report preliminary results using this new wavefunction. We also compare our results with recent calculations obtained using Born-Oppenheimer Molecular Dynamics.

8:36AM A23.00004 First-principles study of the effect of helium on the onset of dissociation in liquid hydrogen , KYLE CASPERSSEN, Lawrence Livermore National Laboratory, FRANCOIS GYGI, University of California Davis, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — The molecular to non-molecular liquid-liquid phase transition that occurs in high-temperature/high-pressure hydrogen has been speculated to be first-order-like, where the onset of dissociation occurs abruptly. However, a small concentration of non-interacting particles, specifically helium, has been postulated to retard and slow the transition. To study this transition in hydrogen and hydrogen-helium mixtures we performed a series of large-scale Born-Oppenheimer molecular-dynamic simulations. Additionally, we have studied the electronic properties of hydrogen-helium mixtures by using hybrid density functional theory to analyze snapshots from our molecular dynamics simulations. The simulations show that the transition is smooth and continuous without any indication of any first-order-like behavior. The simulations also predict that small concentrations of helium have a significant effect on the phase transition; most notably, the pressure profile is much smoother, and the band gap closes at a higher temperature, for the hydrogen-helium mixtures relative to pure liquid-hydrogen. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.
8:48AM A23.00005 Equation of state and electronic structure of liquid Helium at high pressure , LARS STIKRUSE, University of Michigan, RAYMOND JEANLOZ, University of California at Berkeley — As the second most abundant element, the properties of fluid Helium form an important part of our understanding of stellar and giant planetary structure. Yet the physics of Helium at pressure-temperature conditions characteristic of these bodies is uncertain. We perform first principles molecular dynamics simulations of fluid Helium over a wide range of pressure (< 1 Gbar) and temperature (< 5 eV). The simulations are based on finite-temperature density functional theory in the generalized gradient approximation, and are performed in the canonical ensemble with a Nose thermostat. We find that both temperature and compression have a strong influence on the electronic structure as revealed by the band gap. At a density of 1 g cm$^{-3}$ the band gap varies from 20 eV for the static crystal to 0 for the fluid at 4 eV. The gap is closed at all temperatures for density greater than 20 g cm$^{-3}$. We find that the equation of state varies smoothly through the band gap closure transition with no indication of a high-order phase transition. The decrease in band gap with increasing temperature at constant density results from enhanced mixing of 1s- and 2s-like states with increasing disorder (i.e., enhanced vibrational amplitudes and melting) that has profound implications for understanding the deep interiors of planets. [1] V. Iota, et al., Science 283, 1510 (1999).

9:00AM A23.00006 Liquid-liquid transitions in low-Z materials: Parallel with high-pressure solid phase transitions1 . STANIMIR BONEV, ISAAC TAMBLYN, ADAM CHAFFEY, Dalhousie University, Canada. JEAN-YVES RATY, University of Liege, Belgium — First-principles molecular dynamics simulations reported in [1] predict structural and electronic transitions in dense liquid sodium that are responsible for its exotic melting curve. In this talk, the possibility for observing similar behavior in other low-Z materials will be discussed. Results from ab initio calculations of several materials will be presented and compared with sodium. [1] Jean-Yves Raty, Eric Schwegler and Stanimir A. Bonev, submitted.

9:12AM A23.00007 Probing Dense States of Hydrogen and Oxides in Giant Planets using Multiple and Single- Shock Compression and Laser-Pulse-Heated Diamond-Anvil Cells. , W.J. NELLIS, I.F. SILVERA, Harvard University — Pressures and temperatures of hydrogen on adiabats deep in gas giants are achieved using a shock wave reverberating between incompressible oxide anvils and by pulsed heating in a diamond-anvil cell. At 100 GPa in gas giants, temperature varies from ~20,000 K in hot Jupiters down to ~1,000 K in cold Jupiters. The Hugoniot curve of hydrogen crosses these adiabats at ~15 GPa and ~4,000 K for Jupiter and ~100 GPa for hot Jupiters, both at compressions of ~4 fold. Reverberating shocks and diamond cells produce compressions up to ~12 fold. Since dense hydrogen has a huge diffusion coefficient, experiments must be done sufficiently slowly that hydrogen is in thermal equilibrium and sufficiently fast that hydrogen remains in the cell. Dynamic experiments occur within this constraint. DAC experiments require heating by multiple laser pulses each of ~100 ns duration. Pressures and temperatures achieved by multiple shock compression are tuned by variation of the density of oxide anvils. An oxide (Gd$_5$Ga$_2$O$_{12}$) has been found that is stiffer than diamond above 100 GPa. This oxide will enable higher pressures and lower temperatures in metallic fluid hydrogen by multiple shock and might be representative of new oxide phases in deep interiors of giant extrasolar rocky planets. Experiments and systematics will be described.

9:24AM A23.00008 Coherent anti-Stokes Raman Spectroscopy Study of Highly Compressed Deuterium , BRUCE BAER, WILLIAM EVANS, CHOONG-SHIK YOO, Lawrence Livermore National Laboratory — High density (> 0.3 mol/cm$^3$) hydrogen and its isotopes have been studied intensely over the past three decades. Although many spectroscopic methods have been applied, none utilizes a multiphoton technique. Coherent anti-Stokes Raman Spectroscopy (CARS) has now been applied to samples over one megabar for the first time to accurately determine the density at which the bandgap of deuterium is 4.66 eV. This method yields very precise Raman shifts, linewidths and third order polarizability ratios since it avoids the problems associated with strain induced diamond fluorescence above a megabar. The pressure dependent third order polarizability ratios can indicate the location of the bandgap. We will present evidence for extrapolating the metallization pressure using these results and the implications on the phase diagram. This work has been supported by the LDRD and PDRP programs at Lawrence Livermore National Laboratory, University of California under the auspices of the U.S. Department of Energy under Contract No. W-7405-ENG-48.

9:36AM A23.00009 Simple Molecular Systems at High Pressures and Temperatures. , ALEXANDER GONCHAROV, General Geophysical Laboratory, Carnegie Institution of Washington, JONATHAN CROWHURST, LLNL — Knowledge of the elastic, optical and vibrational properties of materials under extreme conditions of high pressure and temperature is crucial for interpreting the results of seismological and planetary observations, for materials science, and for improving our understanding of fundamental physics and chemistry under such conditions. We will present the results of Raman, infrared, and x-ray diffraction measurements of hydrogen, water, nitrogen, and oxygen under conditions of high static pressure and temperature in the diamond anvil cell. High temperatures were generated mainly by laser heating, but also using internal resistive heating. These studies revealed novel phase transitions, complex phase diagrams, unexpected chemical transformations and also helped to established the behavior of interatomic interactions in molecular materials. We thank the following individuals for contributing to this work: N. Goldman, L. Fried, C. Mundy, J. Zaug, R. J. Hemley, E. Gregoryanz, C. Sanloup, M. Somayazulu, Y. Meng, N. Guignot, M. Mezour.

9:48AM A23.00010 Bonding Changes in Compressed Carbon Dioxide: A New Stishovite-like Phase of CO$_2$ , VALENTIN IOTA, Lawrence Livermore National Laboratory — At ambient conditions, carbon dioxide (CO$_2$) is a prototypical molecular system, with strong covalent O=C=O molecular bonds and relatively weak quadrupolar interactions between molecules. At high pressures and temperatures, CO$_2$ transforms to a series of solid polymorphs with differing crystal structures, intermolecular interactions and chemical bonding. In particular, two fully covalent (extended) solid phases have been reported above 40GPa, with characteristics analogous to SiO$_2$ polymorphs. First, CO$_2$-V (above 40GPa and 1500K), consists of a network of corner sharing CO$_4$ tetrahedra and is structurally similar to SiO$_2$ tridymite. And, recently, an extended-solid amorphous phase (a-carbonia), similar to amorphous silica, has been reported at room temperature above 40GPa. Here, we present a new stishovite-like CO$_2$ phase VI, formed by compressing CO$_2$-II above 50GPa and 550K. We define the PT stability domain for the new solid, and present Raman and X-Ray diffraction results consistent with a 6-fold average coordination within a P4$_{2}$/mm structure. Finally, we propose a phase/bonding diagram for carbon dioxide describing the systematic relationship between its molecular and extended phases at high pressures and temperatures. [1] V. Iota, et al., Science 283, 1510 (1999). [2] M. Santoro, et al. Nature 441, 857 (2006).
10:24AM A23.00011 Phase diagram of Nitrogen at high pressures and temperatures1. ZSOLT JENESZ2, JUNG-FU LIN, CHOONG-SHIK YOO, Lawrence Livermore National Laboratory — Nitrogen is a typical molecular solid with relatively weak van der Waals intermolecular interactions but strong intramolecular interaction arising from the second highest binding energy of all diatomic molecules. The phase diagram of solid nitrogen is, however, complicated at high pressures, as inter-molecular interaction becomes comparable to the intra-molecular interaction. In this paper, we present an updated phase diagram of the nitrogen in the pressure-temperature region of 100 GPa and 1000 K, based on in-situ Raman and synchrotron x-ray diffraction studies using externally heated membrane diamond anvil cells. While providing an extension of the phase diagram, our results indicate a “steeper” slope of the $\varepsilon$/$\delta$ phase boundary than previously determined1. We also studied the stability of the $\varepsilon$ phase at high pressures and temperatures. Our new experimental results improve the understanding of the Nitrogen phase diagram. 1. Gregoryanz et al, Phys. Rev. B 66, 224108 (2002)

1This work was performed under the auspices of the US Department of Energy by the University of California, Lawrence Livermore National Laboratory, under contract No. W-7405-ENG-48.

2also at: Stockholm University, Stockholm, Sweden

10:36AM A23.00012 Theoretical precursors to polymeric nitrogen. RAZVAN CARACAS, Bayerisches Geoinstitut, RUSSELL J. HEMLEY, Carnegie Institution of Washington — We predict the existence of new structures of nitrogen based on new observations in analog systems from first-principles density-functional calculations. A series of structures was examined. A structure with orthorhombic symmetry is stable relative to the $\epsilon$ and cubic gauche phases in LDA, whereas GGA shows the $\epsilon$ and the new orthorhombic structure are energetically competitive. This structure is dynamically stable at least from ambient pressure to 90 GPa and thus may be observed as a stable or metastable polynitrogen phase prior to the transition to the atomic phases of nitrogen.

Monday, March 5, 2007 8:00AM - 10:36AM –
Session A27 DMP DCOMP: Focus Session: Computational Nanoscience I-Methods and Applications Colorado Convention Center 301

8:00AM A27.00001 A Hybrid Density Functional Study of SiC Nanotubes1, KAZI ALAM, ASOK K. RAY, University of Texas at Arlington — As a continuation of our previous work on SiC nanoclusters,1 we report here first principles calculations on the electronic and geometric structures of armchair and zigzag silicon carbide nanotubes from (3,3) to (11,11) and (3,0) to (11,0) respectively. The finite cluster approach with dangling bonds terminated with hydrogen has been used. The theoretical formalism used is the hybrid density functional theory incorporating Hartree-Fock exchange with density functional theory exchange-correlation. In particular, we have used the B3LYP hybrid functional and the Los Alamos pseudopotential LANL2DZas implemented in the Gaussian 03 suite of programs. For silicon, the 1s, 2s, and 2p electrons have been represented by core potentials and the remaining electrons as valence states. For carbon and hydrogen, all electron basis sets have been used. A detailed comparison of the structures and stabilities of the systems from first-principles density-functional calculations. A series of structures was examined. A structure with orthorhombic symmetry is stable relative to the $\epsilon$ and cubic gauche phases in LDA, whereas GGA shows the $\epsilon$ and the new orthorhombic structure are energetically competitive. This structure is dynamically stable at least from ambient pressure to 90 GPa and thus may be observed as a stable or metastable polynitrogen phase prior to the transition to the atomic phases of nitrogen.

1This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

8:12AM A27.00002 A Hybrid Density Functional Study of Si Nanotubes1, SOMILKUMAR RATHI, ASOK RAY, Physics Department, University of Texas, Arlington — First principles calculations have been used to study the electronic and geometric structures of zigzag and chiral silicon nanotubes. The finite cluster approach with dangling bonds terminated with hydrogen has been used. The theoretical formalism used is hybrid density functional theory incorporating Hartree-Fock (HF) exchange with density functional theory (DFT) exchange-correlation. In particular, we have used the B3LYP hybrid functional and the Los Alamos pseudopotential LANL2DZ as implemented in the Gaussian 03 suite of programs. For silicon, the 1s, 2s, and 2p electrons have been represented by core potentials and the remaining electrons as valence states. For carbon and hydrogen, all electron basis sets have been used. A detailed comparison of the structures and stabilities of the nanotubes has been performed. The dependence of the electronic band gaps on the respective tube diameters and energy density of states have also been investigated. Results will be compared with other published data in the literature where possible. * A. K. Ray and M. N. Huda, J. Comp. Th. Nanosci. 3, 315 (2006).

1work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

8:24AM A27.00003 Tetra, a modeling system for the generation of the atomic configurations of branched wurtzite/zincblende nanostructures1, PETER GRAF, KWUSEON KIM, WESLEY JONES, National Renewable Energy Laboratory, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The first step in simulating properties of nanostructures is generation of accurate atomic configurations. For complex objects such as the multiply branched heterostructures synthesized by Alivisatos et al.,1 this is nontrivial. We report here on our code, “tetra,” that accomplishes this task. Borrowing from techniques of computer graphics, we represent the complex structure as a tree, each node of which is a shape with fixed crystal structure, and use concatenation of 4 by 4 homogeneous transformation matrices to arrange these fixed building blocks into the final object. A simple text based input “language” describes the connectivity and dimensions of the structure. The ultimate purpose of this code is use within a package that will explore and optimize electronic properties of such structures with respect to their geometry2. We will present examples of both structures and subsequent semi-empirical pseudopotential-based3 electronic structure calculations. [1] A. P. Alivisatos, et al., Nature, 430, 190 (2004). [2] J. Li and L. W. Wang, NanoLetters, 3, 10, 1357-1363 (2003). [3] L. W. Wang and A. Zunger, Phys. Rev. B 51, 17398 (1995).

1This work was supported by US DOE-SC-BES and ASCR TMSN Initiative.
8:36AM A27.00004 Global optimization approaches for finding the atomic structure of surfaces and nanowires. CRISTIAN CIOBANU, Colorado School of Mines — In the cluster structure community, global optimization methods are common tools for seeking the structure of molecular and atomic clusters. The large number of local minima of the potential energy surface (PES) of these clusters, and the fact that these local minima proliferate exponentially with the number of atoms in the cluster simply demands the use of fast stochastic methods to find the optimum atomic configuration. Therefore, most of the development work has come from (and mostly stayed within) the cluster structure community. Partly due to wide availability and landmark successes of scanning tunneling microscopy (STM) and other high resolution microscopy techniques, finding the structure of periodically reconstructed semiconductor surfaces was not generally posed as a problem of stochastic optimization until recently [1], when we have shown that the leading research group for such clusters can have a rather large number of local minima with such low surface energies that the identification of the global minimum becomes problematic. We have therefore set out to develop global optimization methods for systems other than clusters, focusing on periodic systems in one- and two- dimensions as such systems currently occupy a central place in the field of nanoscience. In this talk, we review some of our recent work on global optimization methods (the parallel-tempering Monte Carlo method [1] and the genetic algorithm [2]) and show examples/results from two main problem categories: (a) the two-dimensional problem of determining the atomic configuration of clean semiconductor surfaces [1,2], and (b) finding the structure of freestanding nanowires [3]. While focused on mainly on atomic structure, our account will show examples of how these development efforts contributed to elucidating several physical problems and we will attempt to make a case for widespread use of these methods for structural problems in one and two dimensions.


9:12AM A27.00005 Strained InAs/GaAs quantum structures: non-parabolic simulating model. BRANISLAV VLAHOVIC, North Carolina Central University, Durham NC, 27707, IGOR FILIKHIN, VLADIMIR SUSLOV — A single sub-band model for InAs/GaAs quantum dot (quantum ring), taking into account the strain and piezoelectric potentials, is applied to study the electron spectral properties of QD(QR). The finite confinement band-gap potential is estimated by the band gap difference of the InAs quantum object and the GaAs substrate. An additional potential $V_s (V_s=\text{const for QD, and } V_s=0 \text{ for a substrate})$ is included in the model to simulate the total effect of the strain and piezoelectricity. The non-parabolic approximation is defined by dependence of electron effective mass on the confinement energy according to the Kane formula. The 3D confined energy problem is solved numerically by the finite element method. The adequacy of our model is illustrated by comparing electron energy spectra with ab initio calculations [1]. The experimental data by A. Lorke, et al. (PRL 84 2223 (2000)) for few electrons tunneling into InAs/GaAs QD(QR) are well reproduced within the present model. The non-parabolic effect, which is quite noticeable in our calculations, is also discussed. [1] C. Pryor, PR B 87 1790 (1988); O. Stier, M. Grundmann, and D. Bimberg, PR B 59 5688 (1999); J.I. Climente, J. Planelles, F. Rajadell, J. Phys.: Condens. Matter 17 1573 (2005).

9:24AM A27.00006 Size reduction in layered semiconducting compounds. TIANSHU LI, GIULIA GALLI, Department of Chemistry, University of California, Davis — In the last decade numerous experiments have shown dramatic changes in the optical properties of bulk semiconductors as their size is decreased to nanoscale dimensions. Most investigations have focused on 3D compounds such as II-VI and group IV. A few experiments have also been conducted for layered semiconductors, such as transition-metal dichalcogenides, indicating changes in photoluminescence properties apparently comparable to those found in 3D systems. We present extensive electronic structure calculations of the structural and electronic properties of MoS$_2$ nanostripes and an Aharonov-Bohm loop, taking into account the finite confinement effects of MoS$_2$ nanostripes showing no appreciable quantum confinement effects in single sheet nanoparticles, whose electronic structure is dominated by the surface and in particular edge states near the Fermi level. On the other hand, a strong dependence of the electronic structure is observed as a function of layer stacking and distance. We suggest that the observed photoluminescence variation as a function of size does not pertain to size reduction in single sheets but rather to the number of planes composing the nanoparticle. We also suggest a way to engineer metallic nanowires taking advantage of edge states in nanosheet composites.

9:36AM A27.00007 The design of a nanocontainer for high pressure storage of hydrogen. ZHI-FENG LIU, Chinese University of Hong Kong, DEYAN SUN, East China Normal University, XIANG YE, XINGAO GONG, Fudan University — Molecule hydrogen is known to have a weak van der Waals potential, which makes it difficult to raise its storage efficiency for physiosorption based methods. In this report, we explore the other side of such a weak potential, the well-known compressibility of hydrogen. A (20,0) single wall carbon nanotube based nanocontainer is designed, in which a $C_{60}$ “peapod” at the cap section of the nanotube serves as a molecular valve. Diffusion barriers through such a valve is examined by molecular dynamics simulations under various conditions. It is demonstrated that $H_2$ can first be filled into the container upon compression at low temperature, and then be locked inside it after the release of external pressure. The internal pressure that can be achieved in this design is in the GPa range at room temperature, which is much higher than the typical pressure of a few hundred bar currently employed for hydrogen storage. At 2.5 GPa, the storage weight ratio approaches a promising 7.7%.

1Project supported by RGC, Hong Kong SAR Government.

9:48AM A27.00008 Surface Green functions in molecular transport junctions: The generalization to interacting electrons in the leads. ALEKSEY KLETsov, YURI DAHNOvSKY — The expression for current in transport junctions is generalized to interacting electrons in the leads. We derive a formula for the current where in the expression for line-width matrices the lead density of states is replaced by the surface spectral density matrix for arbitrary $e\cdot e$ interactions in the leads and in the bridge, respectively. This expression is only valid for small lead-bridge interactions. A novel computational method for a surface Green function matrix is introduced to find the surface spectral density (∼ the trace of the imaginary part of the surface Green function matrix). The proposed non-recursive approach results in the solution of the second order equation for the spectral density matrix (the density of states for noninteracting electrons). The single and double principle layer models are studied for aluminum surfaces. We find that the peak in the current at the Fermi level is rather narrow (∼ 2 eV), and can cause a peak in the $I$ matrices resulting in a peak in the current-voltage characteristics. Beside the aluminum surface with fcc-structures, we study a hexagonal structure as well. Such surfaces exhibit a gap and two bands in the spectral density. The gap and the band widths depend on the parameters of the lead Hamiltonian. We show that the narrow gap and the narrow bands can result in large negative resistances in the conduction.

2NFS grant CHE-0426090

10:00AM A27.00009 Adiabatic quantum pumping in an Aharonov-Bohm loop and in a Si-like nanowire: interference in real space and in k-space. SUNGJUN KIM, Department of Physics, The Pennsylvania State University, University Park, PA, KUNAL DAS, Department of Physics, Fordham University, Bronx, NY, ARI MIZEL, Department of Physics, The Pennsylvania State University, University Park, PA — We study interference effects in the current generated by adiabatic quantum pumping in two extended chain models. The first model consists of an Aharonov-Bohm loop within a tight-binding chain of sites. It exhibits interference between the two arms of the loop. We investigate the effect of magnetic field reversal on the pumped current. Our second model is a tight-binding chain of sites with next-nearest-neighbor hopping terms. The resulting Si-like indirect band structure can have 4 degenerate Fermi wave vectors ±$k_F$ and ±$k_P$ rather than the usual 2 Fermi wave vectors ±$k_F$. It exhibits signatures of interference between these degenerate conduction band states.
this background-free measurement possible, and explain how these results can be used to predict \( \Delta \) important probe of electronic structure in aromatic molecules. We will discuss the experimental approach (polarized resonant photoluminescence) that made of fundamental interest. Here we present the first experimental indication of fan-out behavior for orbital magnetic anisotropy (1)

dependence of single-walled carbon nanotube (SWNT) properties often leads to “fan-out” diagrams whose departure from the large diameter scaling limit is anisotropy for arbitrary chiralities (1). The results are consistent with the existence of a dark state below the first bright state (1). In the presence of time reversal symmetry, exchange-interaction-induced mixing between excitons in two equivalent valleys (the K and K' valleys) is expected to result in a set of excitation states, only one of which is optically active. This predicted bright state, however, is not the lowest in energy. Excitons would be trapped in the dark, lowest-energy state without a radiative recombination path. When a tube-threading \( B \) is applied, addition of an Aharonov-Bohm phase modifies the circumferential boundary conditions on the wave functions and lifts time reversal symmetry (2). This symmetry breaking splits the K and K' valley transitions, lessening the intervalley mixing and causing the recovery of the unmixed direct K and K' excitons, which are both optically active. We have calculated PL spectra through \( B \)-dependent effective masses, populations of finite-\( k \) states, and acoustic phonon scattering, which quantitatively agree with the observations. These results demonstrate the existence of dark excitons, their influence on the PL quantum yield, and their elimination through symmetry manipulation by a \( B \). This work was performed in collaboration with J. Shaver, S. Zaric, O. Portugall, V. Krstic, G. L. J. A. Rikken, X. Wei, S. A. Crooker, Y. Miyauchi, S. Maruyama, and V. Perebeinos and supported by the Robert A. Welch Foundation, the NSF, and EuroMagNET.

We have investigated the magnetic field effects on the electronic structure and absorption properties of excitons in single-walled carbon nanotubes (SWNTs), we have studied photoluminescence (PL) from individualized HiPCo and CoMoCAT samples as a function of magnetic field (\( B \)) and temperature (\( T \)). The PL intensity increased, or “brightened,” with \( B \) applied along the tube axis and the amount of brightening increased with decreasing \( T \). These results are consistent with the existence of a dark state below the first bright state (1). In the presence of time reversal symmetry, exchange-interaction-induced mixing between excitons in two equivalent valleys (the K and K' valleys) is expected to result in a set of excitation states, only one of which is optically active. This predicted bright state, however, is not the lowest in energy. Excitons would be trapped in the dark, lowest-energy state without a radiative recombination path. When a tube-threading \( B \) is applied, addition of an Aharonov-Bohm phase modifies the circumferential boundary conditions on the wave functions and lifts time reversal symmetry (2). This symmetry breaking splits the K and K' valley transitions, lessening the intervalley mixing and causing the recovery of the unmixed direct K and K' excitons, which are both optically active. We have calculated PL spectra through \( B \)-dependent effective masses, populations of finite-\( k \) states, and acoustic phonon scattering, which quantitatively agree with the observations. These results demonstrate the existence of dark excitons, their influence on the PL quantum yield, and their elimination through symmetry manipulation by a \( B \). This work was performed in collaboration with J. Shaver, S. Zaric, O. Portugall, V. Krstic, G. L. J. A. Rikken, X. Wei, S. A. Crooker, Y. Miyauchi, S. Maruyama, and V. Perebeinos and supported by the Robert A. Welch Foundation, the NSF, and EuroMagNET.

8:36AM A28.00002 Magnetic field effects on the excitonic absorption spectra of semiconductor single-walled carbon nanotubes

HONGBO ZHAO, University of Hong Kong, ZHENDONG WANG, SUMIT MAZUMDAR, University of Arizona — We have investigated the magnetic field effects on the electronic structure and absorption spectra of semiconductor single-walled carbon nanotubes (S-SWCNTs) within a Coulomb correlated \( e \)-electron model. We consider magnetic field parallel to the nanotube axis, which introduces the Aharonov-Bohm phase in the wavefunction. Recent experiments claim to have observed the energy shift and splitting due to the magnetic field (3). Some of our theoretical results are substantively different from existing results. Comparison with recent experiments are made.

8:48AM A28.00003 Activating Dark Excitons on Carbon Nanotubes with Electric Fields J.M. KINDER, D. ZHABINSKAYA, E.J. MELE, University of Pennsylvania — The valley degeneracy of the singlet excitons on a semiconducting carbon nanotube is lifted by Coulomb backscattering which produces two intervalley superposition states: a bright optically allowed singlet exciton, and a dark (dipole forbidden) singlet exciton at lower energy. We study theoretically the perturbations to this spectrum due to a longitudinal static electric field. We find the electric field transfers oscillator strength from the bright to the dark singlet state and activates the lower energy state in the fluorescence spectrum for modest values of the field strength. Modelling the K and K' point excitons as a two state system, we find that the field induces a complex phase in the intervalley scattering amplitude, which in turn renders the dark state optically active. We study the dependence of this effect on the chiral angle of the tube and further analyze other field configurations that can coherently manipulate the intervalley superposition states produced in this system.

9:00AM A28.00004 ABSTRACT WITHDRAWN

9:12AM A28.00005 Aromatic trends in single-walled carbon nanotubes: diamagnetic anisotropy for arbitrary chiralities O.N. TORRENS, D.E. MILKIE, H.Y. BAN, Dept. of Physics and Astronomy, Univ. of Pennsylvania, M. ZHENG, G.B. ONOA, T.D. GIERKE, DuPont CR&D, J.M. KIKKAWA, Dept. of Physics and Astronomy, Univ. of Pennsylvania — The chirality dependence of single-walled carbon nanotube (SWNT) properties often leads to “fan-out” diagrams whose departure from the large diameter scaling limit is of fundamental interest. Here we present the first experimental indication of fan-out behavior for orbital magnetic anisotropy (\( \Delta \chi \)), which has long been an important probe of electronic structure in aromatic molecules. We will discuss the experimental approach (polarized resonant photoluminescence) that make this background-free measurement possible, and explain how these results can be used to predict \( \Delta \chi \) for arbitrary SWNT chiralities. Taking into account general symmetry considerations, \( ab \) \textit{initio} calculations, large-diameter tight-binding theory, and our experimental data, we obtain a chiral expansion for \( \Delta \chi \) using a single fitting parameter. The results show (2n+m) family trends whose asymmetry between “mod 1” and “mod 2” semiconducting families is reminiscent of those seen in other SWNT optical, phonon, and exciton properties. Finally, we discuss the (n,m) dependence of zone-folding tight binding calculations when applied to realistic tube sizes.

1Supported by NSF DMR-0520020 and DMR-0094156
9:24AM A28.00006 Electron-electron interaction effects on cross-polarized optical absorption in semiconducting single-walled carbon nanotubes (S-SWCNTs)\textsuperscript{1}. ZHENHONG WANG, SUMIT MAZUMDAR, University of Arizona — Within the tight binding theory of S-SWCNTs optical transitions polarized transverse to the nanotube axis, $E_{12}$ and $E_{23}$, are degenerate, and occur at $(E_{11} + E_{22})/2$, where $E_{11}$ and $E_{22}$ are the optical transitions polarized along the nanotube axis. Electron-electron interactions split the degeneracy of the transverse transitions, giving new eigenstates that are a redshifted optically forbidden odd superposition and a blueshifted (by several tenths of 1 eV) optically allowed even superposition of the one-electron excitations\textsuperscript{2}. Recent experiments\textsuperscript{3}\textsuperscript{4} have confirmed our qualitative prediction. Here we report quantitative calculations of the longitudinal versus transverse optical absorptions in the four S-SWCNTs studied by Miyauchi et al., within a $\pi$-electron Hamiltonian with long range Coulomb interactions\textsuperscript{5}. We make detailed comparisons between experiments and theory. We also comment on the role of electron hoppings beyond nearest neighbor and the binding energy of the transverse exciton.

\textsuperscript{1}Supported by NSF-DMR-0406604

9:36AM A28.00007 Dielectric response of aligned semiconducting single-wall nanotubes. B.J. LANDI, RIT, J.A. FAGAN, J.R. SIMPSON, L.J. RICHTER, I. MANDELBAUM, D.L. HO, NIST; R. RAFFAELLE, RIT, A.R. HIGHT WALKER, B.J. BAUER, E.K. HOBBS, NIST — We report measurements of the full intrinsic optical anisotropy of isolated single-wall carbon nanotubes (SWNTs). By combining absorption spectroscopy with transmission ellipsometry and polarization-dependent resonant magnetic scattering, we obtain the real and imaginary parts of the intrinsic SWNT permittivity from aligned semiconducting carbon nanotubes dispersed in stretched polymer films. Our results are in agreement with theoretical predictions, highlighting the limited polarizability of excitons in a quasi-1D system. We discuss the dependence of the measured optical response on nanotube length.

9:48AM A28.00008 Electronic Structure Effects in Single Wall Carbon Nanotubes Dielectric Response. KEVIN TATUR, LILIA WOODS, University of South Florida — The electronic structure of various single wall carbon nanotubes is considered within the sp$^3$ tight-binding model. Parameters for this model are taken from the Slater-Koster model. The sp$^3$ approach is applied in order to take into account the hybridization of the carbon $\sigma$- and $\pi$-orbitals due to curvature of the cylindrical surface of the nanotubes. The curvature dependence of the hopping integrals is also taken into account. Only nearest neighbor interaction is used. The obtained electronic states and energies are then used to calculate the dielectric response of the carbon nanotubes within random phase approximation methods. The real and imaginary parts of the dielectric response function are calculated and the curvature and geometry effects of the different nanotubes are discussed.

10:00AM A28.00009 Bilayer Graphene: An Electrically Tunable Semiconductor. HONGKI MIN, BHAGAWAN SAHU, SANJAY BANERJEE, ALLAN MACDONALD, The University of Texas at Austin — Using ab initio density functional theory calculations, we verify [1,2] that the energy band structure of bilayer graphene can be tuned by applying an external electric field. As the strength of the external electric field increases, the electronic spectrum of bilayer graphene changes from a that of a zero-gap semiconductor to that of a gapped semiconductor. From the ab initio calculations the external field dependence of the screened interlayer potential difference and tunneling amplitudes are extracted by fitting to a tight-binding model. We discuss the role of interlayer correlations in determining the size of the gap and the accuracy of local density approximation. [1] Edward McCann and Vladimir I. Fal’ko, Phys. Rev. Lett. 96, 086805 (2006). [2] Taisuke Ohta, Aaron Bostwick, Thomas Seyller, Karsten Horn, and Eli Rotenberg, Science 313, 951 (2006).

10:12AM A28.00010 Magneto-optical conductivity in Graphene: signatures of the Dirac quasiparticles. SERGEI SHARAPOV, Bogolyubov Institute for Theoretical Physics, JULES CARBOTTE, Department of Physics and Astronomy, McMaster University, VALERY GUSYNIN, Bogolyubov Institute for Theoretical Physics, LILIA WOODS, University of South Florida — The electronic structure of various single wall carbon nanotubes is considered within the sp$^3$ tight-binding model. Parameters for this model are taken from the Slater-Koster model. The sp$^3$ approach is applied in order to take into account the hybridization of the carbon $\sigma$- and $\pi$-orbitals due to curvature of the cylindrical surface of the nanotubes. The curvature dependence of the hopping integrals is also taken into account. Only nearest neighbor interaction is used. The obtained electronic states and energies are then used to calculate the dielectric response of the carbon nanotubes within random phase approximation methods. The real and imaginary parts of the dielectric response function are calculated and the curvature and geometry effects of the different nanotubes are discussed.

10:24AM A28.00011 Excitations from Filled Landau Levels in Graphene\textsuperscript{1}. DREW IYENGAR, JIANHUI WANG, Indiana University, H.A. FERTIG, Indiana University and Technion, LUIS BREY, Instituto de Ciencia de Materiales de Madrid (CSIC), Madrid, Spain — We consider particle-hole excitations of graphene over an integer quantum Hall state. We first analyze the two-body problem of a single Dirac electron and hole in a magnetic field interacting via Coulomb forces. We then turn to the many-body problem, where particle-hole symmetry and the existence of two valleys lead to a number of effects peculiar to graphene. The appearance of different branches in the excition spectrum is sensitive to the filling factor. The coupling together of a large number of low-lying excitations leads to strong many-body corrections, which could be observed in inelastic light scattering or optical absorption.

\textsuperscript{1}Supported by NSF

10:36AM A28.00012 Magneto-plasmon excitations in graphene. GERARD MARTINEZ, GHMF-L-CNRS, Grenoble, France, YURI BYCHKOV, I.D.Landau Institute for Theoretical Physics, Moscow, Russia — Graphene is a monolayer of graphite with a band structure composed of two cones located at two inequivalent corners of the Brillouin zone at which conduction and valence bands merge. In contrast with conventional two dimensional electron gas, the dispersion relation obeys a Dirac law with an energy linear as a function of momentum which leads to a specific square root dependence of the Landau levels under an applied magnetic field. The magneto-optical transitions are either of cyclotron type or valence to conduction type. We derive in this frame the magneto-plasmon picture, for filling factor lower than 2, which should be used to interpret the magneto-optical experiments in this compound.

10:48AM A28.00013 Infrared absorption in graphene. ERIK HENRIKSEN, ZHIGANG JIANG, Columbia University, RICHARD TUNG, YONG-JIE WANG, NHMFL, MOLLIE SCHWARTZ, MELINDA HAN, PHILIP KIM, HORST STORMER, Columbia University — We present evidence for the cyclotron resonance transition between the lowest lying Landau levels near the Dirac point in a single layer of graphene, in magnetic fields up to 18T. At constant field, we modulated the back gate voltage on large area graphene samples to determine the infrared absorption from 400 to 3000 cm$^{-1}$ using a FTIR spectrometer. All data were taken at 4.2K with simultaneous measurement of the graphene carrier densities and mobilities. We find transmission minima having widths of $\approx$ 500 cm$^{-1}$, whose shift in energy is consistent with a square root dependence on the magnetic field as expected for two dimensional Dirac fermions. From this field dependence, the Fermi velocity is estimated at $1.1\times10^7$ m/s, in good agreement with literature values.
8:00AM A42.00001 Quantum size effects in metallic thin films: from thermodynamic stability to superconductivities. CHIH-KANG SHIH, The University of Texas at Austin — In ultra-thin epitaxial metallic film, confinement of electronic states along the vertical direction leads to the formation of quantum well states (QWS). Over the past few years it has been shown that such QWS have profound effects on the thermodynamic stability of thin metal films. It has also been shown that such QWS can modulate local free energy landscape and influence the kinetic processes of mass transport. More recently, evidences that such QWS can also impact collective electronic properties such as superconductivities have also been reported. This talk will focus on direct correlations of all these aspects.

8:36AM A42.00002 Non-classical second layer nucleation in Pb/Si(111) and the kinetics of the wetting layer. M. HUPALO, Ames Laboratory of US DOE, Iowa State University, Z. KUNTOVA, C. Z. WANG, M. C. TRINGIDES, Ames Laboratory of US DOE, Iowa State University — By studying the island growth in stepwise deposition experiments with STM we showed two non-classical features i.e. the unusual second layer ring morphology and the crucial role of the wetting layer in the kinetics. The filling of the vacancy island inside the ring is much slower process than the ring formation due to higher radial diffusion barrier towards the island center. In addition Pb is transferred to unstable islands from the continuous spreading of the wetting layer to the island top uncovering the underlying 7x7 reconstruction. Combined Monte Carlo simulations on a novel Potential Energy Surface (PES) constructed with input from first principles calculation can account for most of these unusual non-classical observations.

8:48AM A42.00003 Quantum Modulation of Island Nucleation on Top of a Metal Nanomesa. YONG HAN, Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112, M. HUPALO, M. C. TRINGIDES, Ames Laboratory of US DOE, Iowa State University, RUI FENG, Georgia Inst. Tech, MICHAEL GRAMLICH, U Missouri-Columbia, EDWARD CONRAD, Georgia Inst. Tech, MAOZHI LI, Ames Laboratory of US DOE, Iowa State University, Z. KUNTOVA, Institute of Physics, Academy of Sciences of the Czech Republic, C. Z. WANG, K. M. HO, M. C. TRINGIDES, Ames Laboratory of US DOE, Iowa State University — By studying the island growth in stepwise deposition experiments with STM we showed two non-classical features i.e. the unusual second layer ring morphology and the crucial role of the wetting layer in the kinetics. The filling of the vacancy island inside the ring is much slower process than the ring formation due to higher radial diffusion barrier towards the island center. In addition Pb is transferred to unstable islands from the continuous spreading of the wetting layer to the island top uncovering the underlying 7x7 reconstruction. Combined Monte Carlo simulations on a novel Potential Energy Surface (PES) constructed with input from first principles calculation can account for most of these unusual non-classical observations.

9:00AM A42.00004 In situ x-ray scattering investigation of the Pb/Si(111)7x7 interface. MICHAEL GRAMLICH, U Missouri-Columbia, RUI FENG, Georgia Inst. Tech, SHAWN HAYDEN, U Missouri-Columbia, MYRON HUPALO, MICHAEL TRINGIDES, Ames Laboratory, CHINKYO KIM, KyungHee U, M. C. TRINGIDES, Ames Laboratory, M. HUPALO, U Missouri-Columbia, K. M. HO, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — A rapid coarsening behavior was observed experimentally for Pb islands grown on Si(111) surface. It was found that quantum size effects lead to the breakdown of the classical Gibbs-Thomson analysis for this novel behavior. Here we propose a rate equation model where quantum size effects are incorporated by introducing an appropriate dependence of the chemical potential of Pb islands on their heights as well as on their curvatures. The evolution of the chemical potential of the wetting layer between islands is estimated, we also estimate the mesa edge barriers for the 5- and 6-layer Pb(111) mesas can differ by ~23 ± 7 meV.

9:12AM A42.00005 Strongly-Driven Coarsening of Height-Selected Pb Islands on Si(111). MAOZHI LI, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, J. W. EVANS, Ames Laboratory and Department of Mathematics, Iowa State University, C. Z. WANG, M. HUPALO, M. C. TRINGIDES, T.-L. CHAN, K. M. HO, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — A rapid coarsening behavior was observed experimentally for Pb islands grown on Si(111) surface. It was found that quantum size effects lead to the breakdown of the classical Gibbs-Thomson analysis for this novel behavior. Here we propose a rate equation model where quantum size effects are incorporated by introducing an appropriate dependence of the chemical potential of Pb islands on their heights as well as on their curvatures. The evolution of the chemical potential of the wetting layer between islands is also incorporated. It is shown that rate equations predict evolution of the island density and height distribution in good agreement with experiments.

9:24AM A42.00006 Stability of magic planar Ag clusters. Y.P. CHIU, Department of Physics, National Sun Yat-sen University, Y.S. OU, Y.R. CHANG, Institute of Physics, Academia Sinica; Department of Physics, National Taiwan University, C.M. WEI, Institute of Atomic and Molecular Sciences, Academia Sinica; Institute of Physics, Academia Sinica; Institute of Physics, Academia Sinica, C.S. CHANG, TIEN T. TSONG, Institute of Physics, Academia Sinica — The spontaneous assembly of atoms and molecules in a system has attracted many research interests and created numerous potential applications. Utilizing the periodic pattern found on the Pb quantum islands, which are grown on the Si(111) surface, we have recently discovered that self-organized Ag planar clusters formed on these templates exhibit enhanced stability at some particular sizes. Existence of the magic atom numbers in these clusters is mainly attributed to the electronic confinement effect. Here, we further explore the strength of these magic clusters subject to the temperature rise and oxygen exposure. Detailed calculations based on ab initio density functional theory have also been performed. The results help establish the relation between the physical and chemical stability of a magic Ag cluster and its size and shape. Ref:[1] Ya-Ping Chiu, Li-Wei Huang, Ching-Ming Wei, Chia-Seng Chang, and Tien-Tzou Tsong, Phys. Rev. Lett. 97, 165504 (2006).
9:36 AM A42.00007 Self Organization of Pb Islands on Si(111) Caused by Quantum Size Effects, HAWOONG HONG, University of Illinois, Urbana-Champaign, LEO BASILE, Escuela Politécnica Nacional, PETER CZOSCHKE, Seagate Technology, AARON GRAY, TAI-CHANG CHIANG, University of Illinois, Urbana-Champaign — Growth of metallic Pb islands on Si(111) by vacuum deposition was studied in real time using synchrotron x-ray diffraction. The islands coarsen and order, maintaining a nearly uniform inter-island distance but without angular correlation. The resulting inter-island structure is akin to a two-dimensional liquid. Over a wide temperature range, the inter-island ordering is well correlated with the development of “magic” island heights caused by energy minimization of the Pb electrons. The results demonstrate quantum confinement effects as a driving force for self-organization, as opposed to strain effects that generally govern the formation of semiconductor quantum dot arrays.

9:48 AM A42.00008 First-principles Study of Pb(111) Nanofilms in the Quantum Regime1, YONG HAN, RAJ GANESH S. PALA2, GUANG-HONG LU3, Department of Material Science and Engineering, University of Utah, Salt Lake City, UT 84112-0610, USA, LI HUANG4, Surface Physics Laboratory and Department of Physics, Fudan University, Shanghai 200433, P. R. China, FENG LIU, Department of Material Science and Engineering, University of Utah, Salt Lake City, UT 84112-0610, USA — We report first-principles calculations to investigate surface free energy, interlayer spacing, surface stress, and surface self-diffusion barrier for Pb(111) films in the thickness range of 1 to 31 monolayers, where the quantum size effect (QSE) dominates. We show that similar to surface free energy, all these properties exhibit an oscillation behavior and a beating pattern as a function of film thickness. We will discuss correlations between these properties in terms of QSE.

1This work is supported by NSF.
2Current address: Department of Chemistry and Biochemistry University of California, Santa Barbara, CA 93106-9510, USA
3Current address: School of Science, Beihang University, Beijing 100083, P. R. China
4Current address: School of Physics, Georgia Institute of Technology, Atlanta, GA 30332-0430, USA

10:00 AM A42.00009 Strength modulation of quantum-well states in Pb islands with periodic distortions, S.M. LU, M.C. YANG, W.B. SU, C.L. JIANG, C.S. CHANG, TIEN T. TSONG, Institute of Physics, Academia Sinica, Taiwan, R.O.C. — We use scanning tunneling microscopy and spectroscopy to reexamine the system of three-atomic-layer Pb islands with two types of patterns grown on Si(111) surface. Our results demonstrate that the pattern on the island surface appears as the superposition of geometric corrugaion and local variation of the electronic structure. The former originates from two kinds of interfacial relaxations, resulting in two types of periodic distortions in the Pb layer. The latter is due to the periodic strength modulation of quantum-well states in Pb islands, causing inequivalence in the integration of the density of states, and the pattern is bias-dependent. This strength modulation of the quantum-well states can be correlated to the electronic screening effect induced by the lattice distortion in Pb islands.

10:12 AM A42.00010 Coherent Electronic Fringe Structure in Incommensurate Silver-Silicon Quantum Wells, NATHAN SPEER, SHU TANG, TOM MILLER, TAI CHIANG, University of Illinois at Urbana-Champaign — Atomically uniform Ag films grown on highly doped n-type Si(111) substrates show fine-structured electronic fringes near the Si valence band edge as observed by angle-resolved photoemission. No such fringes are observed for Ag films grown on lightly doped n-type substrates or p-type substrates, although all cases exhibited the usual quantum well states corresponding to electron confinement in the film. The fringes correspond to electronic states extending over the Ag film as a quantum well and reaching into the Si substrate as a quantum slope, with the two parts coherently coupled through an incommensurate interface structure.

10:24 AM A42.00011 First-principles studies of quantum growth of PbBi alloy films1, YU JIA, Zhengzhou University, M. M. OZER, JAMES R THOMPSON, H. H. WEITERING, The University of Tennessee, ZHENYU ZHANG, ORNL — Quantum growth of Pb0.89Bi0.11 alloy films freestanding or grown on Si(111) and Ge(111) substrates has been studied using first-principles calculations within density functional theory. Our studies show that the surface energy, work function, and lattice relaxation of the quantum alloy films all oscillate strongly with the film thickness. Similar to the case of pure Pb(111) films, the oscillation pattern is bayer, interrupted with even-odd crossovers. However, the positions of the crossovers and the beating periodicity can be tuned by the contents of Bi in the alloys, with the beating periodicity given by 13ML, 15ML and 17ML for Pb0.89Bi0.11, Pb0.86Bi0.14 and Pb0.75Bi0.25, respectively. These results are in quantitative agreement with experiment.

1Supported by NSF of China, the BES program of the US DOE, and US NSF.

10:36 AM A42.00012 Umklapp-Mediated Quantization of Electronic States in Ag Films on Ge(111), SHU-JUNG TANG, YEN-RU LEE, SHIH-LIN CHANG, National Tsing Hua University, THOMAS MILLER, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign — We employ angle-resolved photoemission to study the electronic structure of atomically uniform films of Ag grown on Ge[111]. A new kind of quantum well state is observed near a specific emission direction away from the surface normal. In contrast with the usual quantum well state arising from electron confinement by specular reflections at the surface and interface of the film, the new kind involves retroreflections, or umklapp reflections, at the interface. It requires four reflections, instead of the usual two reflections, to complete a coherent interference path.

10:48 AM A42.00013 The Phases of Ag on Ge(111): A Low Energy Electron Microscopy Investigation, JASON GIACOMO, SHIRLEY CHIANG, University of California, Davis — The phases of Ag on Ge[111] have been investigated with low energy electron microscopy (LEEM). We have studied the growth of the well known (4x4) and (√3x√3)R30° phases of Ag. LEEM images show the (4x4) phase grows on the surface with a high dependency on surface steps. The (√3x√3)R30° phase then grows as the Ag concentration increases with little dependence on the steps. These features are explained by the diffusivity of Ag on the surface. LEEM has also been used to study the phase transitions at the Ag desorption temperature. Video rate data shows an interesting phase transition as small domains of Ag abruptly change from the (√3x√3)R30° to the (4x4) phase and then from the (4x4) to a disordered 2D gas phase. Although the disordered phase shows no contrast in the LEEM images we know it exists because as the sample is cooled down the remaining Ag on the surface condenses back into the (4x4) and (√3x√3)R30° phases depending on how much Ag has desorbed.

Monday, March 5, 2007 8:00AM - 11:00AM — Session A43 FIAP DMP: Focus Session: Physics of Thermoelectric Materials and Phenomena
Searching for new Thermoelectric Materials from Theory

8:00AM A43.00001 Searching for new Thermoelectric Materials from Theory. WENQING ZHANG, State Key Lab of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China — Thermoelectric (TE) materials are a type of energy materials that can be applied to directly convert waste heat into electricity. Research on advanced TE materials has been a worldwide focus in recent years. By employing density functional \textit{ab initio} methods, we are trying to find new compounds with promising TE performance. In this talk, the following topics will be mainly covered. 1) General discussion on the directions of searching for new TE compounds with good performance; 2) Filling fraction limits (FFLs) for filler impurities in CoSb$_3$. By combining \textit{ab initio} calculations and thermodynamic consideration, we explained the FFLs, revealed the physical mechanism behind FFLs, and found a simple rule for selecting new filler atoms. A few new filled skutterudites with ultra high filling fractions of impurities were predicted theoretically and synthesized experimentally, and they do show promising thermoelectric performance.

3) Rare-earth-related Half-Heusler compounds are used as model systems to discuss the effect of localized electronic states on thermoelectric performance. By that, we will partially discuss the possibility of going beyond narrow-gap materials for thermoelectrics.

Work supported by National 973 project under Grant No. 2007CB607503 and National Science Foundation of China under Grant No. 50672118.

8:36AM A43.00002 Atomic Ordering and Gap Formation in Ag-Sb Based Ternary Chalcogenides. S. M. MALHANTI, KHANG HOANG, JAMES R. SALVADOR, Michigan State University, MERCOURI G. KANATZIDIS, Northwestern University — Ag-Sb based ternary chalcogenides are important in optical phase change and thermoelectric applications. Although discovered almost 50 years ago and thought to be semiconductors, a fundamental understanding of their electronic structures had been lacking. We report \textit{ab initio} electronic structure studies using density functional theory (DFT) to explain their observed atomic structures, the physics of gap formation and their low-energy properties.

Total energy calculations yield theoretical atomic structures which are consistent with experiment. Ag/Sb ordering is found to have a huge impact on the electronic structure near the Fermi energy. It gives pseudogap structure in some ordered structures, and either a pseudogap or a gap in others. For the lowest energy structures, as one goes from Te to Se to S, the (indirect) band gap goes from being negative to positive. Transport properties of Ag$_2$Sb$_2$Te$_5$ can be understood in terms of a small intrinsic band gap and extremely shallow impurity states. The calculated negative band gap in this compound can be ascribed to the deficiency of DFT.

Work partially supported by ONR-MURI Grant No. N00014-03-10789.

8:48AM A43.00003 First-principles Studies of ErAs and ErAs/GaAs Heterostructures. KRIS T. DELANEY, NICOLA A. SPALDIN, CHRIS G. VAN DE WALLE, Materials Research Laboratory, UC Santa Barbara — We present a computational investigation of the materials properties of rare-earth pnictides. ErAs, a semimetal with rock-salt structure, has been demonstrated to grow epitaxially on GaAs substrates with a continuous As sublattice and low strain. The electronic structures have the potential to provide high-quality thermoelectric materials. Using plane-wave based density-functional methods we have performed a detailed investigation of the effects of $f$ electrons on the electronic and atomic structure, using both norm-conserving pseudopotentials and the projector-augmented-wave method. Our preliminary results indicate that it is possible to obtain an adequate description of the band structure without having to include the $f$ electrons as valence electrons. The resulting reduction in computational complexity allows us to perform open explicit simulations of heterostructures. We have also calculated deformation potential constants, to be used in detailed comparisons with experiments where strain affects the band structure.

9:00AM A43.00004 Electronic and vibrational properties of the Na$_{16}$Rb$_8$Si$_{136}$ and K$_{16}$Rb$_8$Si$_{136}$ clathrates. KOUSHIK BISWAS, CHARLES W. MYLES, Department of Physics, Texas Tech University — We have studied the electronic and vibrational properties of the Na$_{16}$Rb$_8$Si$_{136}$ and K$_{16}$Rb$_8$Si$_{136}$ clathrates, using the local density approximation. In qualitative agreement with the rigid-band model, the electronic band structures display no major modifications due to inclusion of the alkali metal guests. However, the electronic densities of states show two sharply peaked structures and a dip near the Fermi level. This feature may help to qualitatively explain the temperature dependent Knight shift observed for the NMR active nuclei in Na$_{16}$Rb$_8$Si$_{136}$. Phonon dispersion curves show low frequency, localized \textquote{grattler} h modes for both clathrates. These modes may efficiently scatter the heat carrying host acoustic phonons, potentially suppressing the lattice thermal conductivity. Based on the harmonic oscillator model and on our calculated rattler frequencies, we predict the isotropic mean square displacement amplitude (U$_{iso}$) of the various guests in these clathrates. Our predicted values of U$_{iso}$ for Na and Rb in Na$_{16}$Rb$_8$Si$_{136}$ are found to be in good agreement with experiment.

9:12AM A43.00005 Theoretical study of lattice thermal conductivity in Si clathrate materials. JIANJUN DONG, XIAOLI TANG, Physics Department, Auburn University — Recent experiments have shown that Si and Ge clathrate crystals are promising candidates as high ZT thermoelectric materials because of their glass-like low thermal conductivity. Based on a detailed \textit{ab initio} calculation of equilibrium statistical properties, we conclude that the distinct structural differences in the equilibrium thermal properties in the two tetrahedrally bonded Si phases. In this talk, we will present our recent calculations of non-equilibrium thermal transport properties of d-Si and Si$_{136}$ crystals, based on the statistical linear response theory. The key step of our calculation of lattice thermal conductivity ($\kappa$) is to evaluate the fluctuation-correlation relation of bulk heat currents at equilibrium conditions. In the current study, we have adopted the molecular dynamics (MD) simulation techniques, using large atomic supercell models and the Tersoff potential. Our results suggest that the cage-like open framework of clathrate crystals will lead to a factor of 5-8 reduction in thermal conductivity. The MD simulation results are also discussed in the context of the simple kinetic transport model. The \textquote{anomalous} oscillation feature in the correlation functions of clathrate materials is explained.


1Petroleum Research Fund
9:36AM A43.00007 First principles Theory of the Lattice Thermal Conductivity of Si and Ge
D. A. BROIDO, Boston College, M. MALORNY, University of Regensburg, N. MINGO, CEA-Grenoble and University of California at Santa Cruz, D. A. STEWART, Cornell University — The room temperature lattice thermal conductivity of high quality crystalline semiconductors is limited by the scattering between phonons arising from the anharmonicity of the interatomic potential. We have calculated the lattice thermal conductivity of isotopically enriched silicon and germanium, combining a first principles approach to extract the harmonic and anharmonic interatomic force constants [1] with an iterative solution of the full Boltzmann-Peierls equation for phonon transport [2]. Our calculated lattice thermal conductivities for Si and Ge, obtained with no adjustable parameters, show a very good agreement with measured values [3,4] and a marked improvement to results obtained previously using empirical interatomic potentials [2].


9:48AM A43.00008 Three-Phonon Phase Space as an Indicator of the Lattice Thermal Conductivity in Semiconductors
L. LINDSAY, D. A. BROIDO, Boston College — The room temperature lattice thermal conductivity of many semiconductors is limited primarily by three-phonon scattering processes arising from the anharmonicity of the interatomic potential. We employ an adiabatic bond charge model [1,2] for the phonon dispersions to calculate the phase space for three-phonon scattering events of several group IV and III-V semiconductors. We find that the amount of phase space available for this scattering in materials varies inversely with their measured thermal conductivities. Anomalous behavior occurs in III-V materials having large mass differences between cation and anion, which we explain in terms of the severely restricted three-phonon phase space arising from the large gap between acoustic and optic phonon branches.


1Supported in part by the Petroleum Research Fund

10:00AM A43.00009 Monte Carlo Simulation of Thermal Conductivity in Randomly Distributed Nanowire Composites
W. TIAN, R. YANG, Dept. of Mech. Engr., Univ. of Colorado, Boulder — In this paper, we investigated the thermal conductivity of composites made of two types of randomly stacked nanowires with high contrast ratio of bulk thermal conductivity. Thermal conductivity predictions based on solving the phonon Boltzmann transport equation by using the Monte Carlo method are presented for different contrast ratios of thermal conductivity, sizes of nanowires and the volumetric fractions in the composites. For composites made of nanowires with high contrast ratio thermal conductivity, the thermal conductivity of the nanocomposites increase dramatically when the volumetric fraction of high thermal conductivity nanowire is higher than the geometry percolation threshold, although existing correlations in percolation theory do not fit the results due to the phonon interface scattering. On the other hand, when the size of nanowires is small and the volumetric fraction of high thermal conductivity nanowire is less than percolation threshold, the thermal conductivity of the nanocomposites decreases with increasing the volumetric fraction of the high thermal conductivity nanowires. The results of this study may help the development of nanoscale thermoelectric materials in which the figure of merit is optimized by choosing appropriate nanowire size, property contrast and composition. RY acknowledges the funding support for this work by DoD/AFOSR MURI grant FA9550-06-1-0326. The simulation was conducted on a 24-node cluster supported by Intel Corporation and managed by Prof. Gang Chen and Mr. Lu Hu at MIT.

10:12AM A43.00010 Optimized thermal conductivities of Silicon Germanium nanowires
JOHN REED, ANDREW WILLIAMSON, GIULIA GALLI, Lawrence Livermore National Laboratory, YING MENG, MUELLER TIM, CEDER GERBRAND, Massachussets Institute of Technology — The measure of the thermoelectric efficiency of a material is given by its “Figure of merit” (Z), which is inversely proportional to its thermal conductivity, and directly proportional to its electrical conductivity. Alloys of Si and Ge are promising thermoelectric materials, since they can be engineered so as to have a low thermal conductivity relative to their electrical conductivity. We present molecular dynamics simulations of the thermal conductivities of Si$_x$Ge$_{1-x}$ nanowires, and an optimization strategy to obtain maximal values of ZT for these systems. We found that Si-Ge alloy nanowires have a significantly lower thermal conductivity than pure Si or Ge nanowires of the same diameter. Furthermore the alloy ordering is found to significantly effect thermal conductivities, and hence is a key parameter to control and vary in order to optimize thermal conductivities and eventually Z values. Towards this end optimal orderings of Si and Ge for low thermal conductivities have been predicted. This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

10:24AM A43.00011 First Principles Studies of Thermoelectric Figure of Merit of Si and SiGe Nanowires
TRINH VO, JOHN REED, ANDREW WILLIAMSON, Lawrence Livermore National Laboratory, YING MENG, TIM MUELLER, MARIA CHAN, GERBRAND CEDER, Massachusetts Institute of Technology, GALLI GIULIA, University of California at Davis, LAVENRE LIVERMORE NATIONAL LABORATORY TEAM, MASSACHUSETTS INSTITUTE OF TECHNOLOGY COLLABORATION, UNIVERSITY OF CALIFORNIA AT DAVIS COLLABORATION — We present predictions of the thermoelectric figure of merit (ZT) of Si$_x$Ge$_{1-x}$ nanowires based on Density Functional Theory calculations and cluster expansion optimizations. The electrical conductivity, $\sigma$, and Seebeck coefficient, S, were obtained using the Boltzmann transport equation in the relaxation time approximation, and first principles, electronic structure calculations. The thermal conductivity was computed using classical molecular dynamics runs. A range of SiGe nanowires with different Ge concentrations and Ge distributions were investigated. We found that the transport coefficients $\sigma$, S, and thus ZT strongly depend on the wire growth direction, surface structure, and Ge concentration, and Ge distribution. These parameters were varied to obtain a nanostructure with an optimal, high figure of merit above 2 or 3, depending on the electronic doping.

This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

10:36AM A43.00012 Calculation of figure of merit for Bi$_5$Te$_3$ nanostructures
FABIANO OYAFUSO, Jet Propulsion Laboratory, SMITH NIELSEN, California Institute of Technology, SEUNGWON LEE, Jet Propulsion Laboratory, JAMIL TAHIR-KHELI, California Institute of Technology, PAUL VON ALLMEN, Jet Propulsion Laboratory, WILLIAM GODDARD III, California Institute of Technology — Bi$_5$Te$_3$-based materials comprise one class of promising candidates for novel thermoelectric devices, for which low/high thermal/electrical conductivity are desired. We shall present calculations highlighting the effects of reduced dimensionality on the thermoelectric figure of merit ZT for such materials, with particular emphasis on Bi$_5$Te$_3$ / Sb$_2$Te$_3$ superlattices. The calculation consists of two components, a tight-binding electronic calculation for the electrical conductivity and electronic contribution to the thermal conductivity and a Green-Kubo molecular dynamics approach for the lattice contribution to the thermal conductivity.

1Supported by DARPA.
Non-equilibrium thermoelectric transport in thin film heterostructures1, MONA ZEBARJADI, ALI SHAKOURI, KEIVAN ESFARJANI, University of California, Santa Cruz — The Monte Carlo technique is used to calculate thermoelectric transport properties across thin-film heterostructures. We study the size and position dependence of the Seebeck coefficient across a thin film InGaAsP barrier layer sandwiched between two InGaAs contact layers. With decreasing size, the effective Seebeck coefficient is increased. The transition between pure ballistic thermionic transport and fully diffusive thermoelectric transport is described. We characterized the non-equilibrium length of the device and deduce the power dissipated to the lattice.

1This work was supported by ONR MURI Thermionic Energy Conversion center

Monday, March 5, 2007 8:00AM - 11:00AM —
Session A44 DMP: Focus Session: Nanoscale Transport - Wires, Dots, Point Contacts Colorado Convention Center 507

Time Resolved Characterization of Tunneling in a Quantum Dot, KENNETH MACLEAN, SAMI AMASHA, IULIANA RADU, MIT, DOMINIK ZUMBUHL, University of Basel, MARC KASTNER, MIT, MICAH HANSON, ARTHUR GOSSARD, UCSB — Measurements are presented of the rates for tunneling on and off a laterally defined GaAs quantum dot as a function of drain source bias, plunger gate voltage, and magnetic field. The measurements are obtained using a quantum point contact as a real-time charge sensor, and utilizing pulsed gate techniques. In zero magnetic field, we find evidence that the tunneling is elastic, and that the observed exponential dependences of the tunneling rates on drain-source bias and plunger gate voltage agree quantitatively with a model that takes into account changes in the electron energy relative to the top of the tunnel barrier. In a magnetic field applied parallel to the two dimensional electron gas, we resolve contributions to the tunneling from the two Zeeman sublevels, and discuss how the magnetic field modifies the tunneling rates. This work has been supported by the ARO (W911NF-05-1-0062), the NSF (DMR-0353209), and in part by the NSEC Program of the NSF (PHY-0117795).

Charge Transitions in a Quantum Dot Induced by an Adjacent Quantum Point Contact, S. AMASHA, K. MACLEAN, MIT, D. M. ZUMBUHL, U. Basel, I. P. RADU, M. A. KASTNER, MIT, M. P. HANSON, A. C. GOSSARD, UCSB — Quantum point contact (QPC) charge sensors have become an important tool for measuring the occupation of laterally gated quantum dots in AlGaAs/GaAs heterostructures. However, electrical fluctuations across the QPC have been shown to induce changes in the dot occupation. Using real-time charge detection techniques, we observe this effect in the increased rates at which electrons tunnel on and off the dot with increasing bias applied across the adjacent QPC. Applying an in-plane magnetic field splits the orbital states by the Zeeman energy. We present measurements of the probability of being in the excited spin state after a large bias pulse is applied across the QPC. We propose that changes in dot occupation can qualitatively account for an observed enhancement in the probability of being in the excited spin state. This work is supported by the ARO (W911NF-05-1-0062), the NSF (DMR-0353209) and in part by the NSEC Program of the NSF (PHY-0117795).

Interpretation of Fano lineshape reversal in quantum waveguides1, H.R. SADEGHPOUR, Harvard-Smithsonian CFA, Cambridge, MA 02138, N. MOISEYEV, S. KLAIMAN, Dept of Chemistry - Technion Institute of Technology, Haifa, Israel — Fano lineshape parameter (q) reversal is a proxy for interaction beyond the usual interference of indistinguishable quantum pathways. Reversal of the Fano parameter has been observed recently in quantum dots (QD). We show that such a profile reversal may come about from the interaction of interlopping over-the-top states (shape resonances) in the “non-resonant” channel with the QD bound states, interacting with the continuum channel (Feshbach resonances). Using this mechanism we show that with minimal modifications of the QD parameters, we can affect the presence or absence of interloping resonances and hence lineshape profile reversal, as a way of coherence engineering.

1National Science Foundation

Spontaneous Spin Polarization in Quantum Point Contacts, LEONID ROKHINSON, Purdue University — Mesoscopic systems exhibit a range of non-trivial spin-related phenomena in the low density regime, where inter-particle Coulomb interactions become comparable to their kinetic energy. In zero-dimensional systems spontaneous polarization of a few-electron quantum dot leads to a spin blockade, a remarkable effect where mismatch of a single spin blocks macroscopic current flow. In two-dimensional hole gases there is an experimental evidence of a finite spin polarization even in the absence of a magnetic field. In one-dimensional systems quantum wires and quantum point contacts - a puzzling so-called “0.7 structure” has been observed below the first quantization plateau. Experiments suggest that an extra plateau in the conductance vs gate voltage characteristic at 0.7 × 2e2/h is spin related, however, the origin of the phenomenon is not yet understood and is highly debated. We report direct measurements of finite polarization of holes in a quantum point contact (QPC) at conductances G < 2e2/h [1]. We incorporated QPC into a magnetic focusing device so that polarization can be measured directly using a recently developed spatial spin separation technique [2]. Devices are fabricated from p-type GaAs/AlGaAs heterostructures. A finite polarization is measured in low-density regime, when conductance of a point contact is tuned to < 2e2/h. We found that polarization is stronger in samples with well defined "0.7 structure".


9:12AM A44.00005 “0.7” Conductance Anomaly in quantum point contacts1, J. SHABANI, R.N. BHATT, Department of Electrical Engineering, Princeton University — We demonstrate that an anomaly close to 0.7(2e2/h) rather than 0.5(2e2/h) as in a Kondo-type model1 in the conductance plot of quantum point contacts2 arises naturally in a model with a quasi-bound state at the Fermi level within an Anderson impurity model framework. The same model yields good agreement with the observed dependence3 of conductance with gate voltage, magnetic field, temperature and also with the observed zero bias anomaly. Further implications within this model are explored and contrasted with other proposed explanations of the anomaly1.


1Supported by NSF-MRSEC (DMR-0213706) and DOE.
9:24AM A44.00006 Spin-orbit induced spin-density wave in a quantum wire. SUHAS GANGADHARAI, JIANMIN SUN, OLEG STARYKH, University of Utah — We consider an interacting quantum wire in the presence of a magnetic field and spin-orbit interaction. We show that under a subtle interplay of magnetic and spin-orbit terms, new scattering channels open up when the magnetic field and the spin-orbit axes are orthogonal: two electrons with opposite momentum and in the same spin-subband scatter into a different spin-subband while conserving momentum. This scattering process is relevant and results in a spin-density wave (SDW) state. We next analyze charge transport property in a scenario when the SDW state survives the presence of a single weak impurity. We find that the single particle back-scattering off a non-magnetic impurity becomes irrelevant. The sensitivity of the SDW state, and hence the charge transport, to the mutual orientation and magnitude of the magnetic and spin-orbit terms can be used for the experimental verification of this novel field and spin-orbit induced state.

9:36AM A44.00007 Suppression of Landau level spin splitting in quantum point contacts. IULIANA RADU, MIT, J.B. MILLER, E. LEVENSON-FALK, Harvard U., S. AMASHA, MIT, D.M. ZUMBühl, U. Basel, M.A. KASTNER, MIT, C.M. MARCUS, Harvard U., L.N. PFIEFFER, K.W. WEST, Bell Labs, Lucent — We investigate low temperature transport properties of split-gate devices lithographically patterned on a GaAs/AlGaAs heterostructure containing a 2D electron gas with mobility 2000 m²/Vs in a perpendicular magnetic field. By using quantum point contacts (QPCs) with different lithographic widths and varying the voltage applied on the gates for each QPC, we can control the width of the conduction channel continuously from ~3000 to ~100nm. The width of the channel is estimated from the low-field magnetic field dependence of the conductance through the QPC. We find that the spin-splitting of the Landau levels is suppressed in the QPCs compared to the bulk, and we measure the filling factor ν_max above which spin splitting can no longer be observed. Surprisingly, we find that ν_max is approximately half the number of quantum channels in the QPC for all widths less than 1200 nm. This work was partially supported by ARO (W911NF-05-1-0062), by the NSEC program of NSF (PHY-0117795), by NSF (DMR-0353209) and by Project Q of Microsoft.

9:48AM A44.00008 Effect of a strong spin-charge separation on tunneling into a 1D wire with impurity. ANDREW MEYERTHOLEN, LINGFENG ZHANG, MICHAEL FOGLER, UCSD — We analyze the tunneling of electrons into a 1D nanowire with a large difference in velocities of spin and charge excitations: charges are “fast,” spins are “slow.” This system is modeled as a Wigner crystal of charges whose spins are ordered as in a antiferromagnetic Heisenberg spin chain. If the wire contains an impurity, electron tunneling in its vicinity causes a novel type of the orthogonality catastrophe. The tunneling electron shifts the charge distribution of a Wigner-crystal, which causes a shake-up processes in the spin sector. The corresponding suppression of the tunneling has a novel temperature dependence, which can be used for an experimental validation of the spin-charge separation in low-density nanowires.

10:00AM A44.00009 Quantum Dots on Silicon Nanowires. HYUK JU RYU, JEREMY HIGGINS, PINRAY HUANG, JEREMY STREIFER, ROBERT HAMERS, SONG JIN, MARK ERIKKSON, University of Wisconsin-Madison — Silicon nanowires have single-crystal structure, well-controlled doping, and can be integrated into devices using either directed assembly and dielectrophoresis or electron-beam lithography and lift-off. Such nanowires, with nanometer size in two dimensions, provide advantages for the fabrication of ultra-small silicon quantum dots with potentially long spin coherence times. We present methods for the fabrication of silicon nanowire-based single electron transistors, and we show results of both room temperature and low temperature transport measurements. The metal electrode structure and annealing process have been intensively investigated to obtain the necessary contact properties. Either metal/nanowire contacts or electrostatically depleted regions have been used for tunneling barriers for quantum dots. Coulomb blockade has been demonstrated successfully, showing 1.3 aF and 1.1 meV for the gate capacitance and the charging energy respectively. Studies of double quantum dots and spin-dependent effects are ongoing.

1 This work has been supported by NSF NSEC program (DMR-0425880).

10:12AM A44.00010 Ballistic hole transport and spin-orbit effects in GaAs quantum wires. ALEX HAMILTON, R. DANNEAU, O. KLOCHAN, W.R. CLARKE, A.P. MICOLICH, L.H. HO, M.Y. SIMMONS, University of New South Wales, M. PEPPER, D.A. Ritchie, University of Cambridge, K. MURAKI, Y. HIRAYAMA, NTT Basic Research Laboratories, U. ZUELICKE, Massey University — Studying the spin degree of freedom of charge carriers in semiconductors has become an area of significant current interest. Although spin-orbit coupling is extremely strong in p-type semiconductors such as GaAs, to date there have been only a limited number of experiments on holes in p-GaAs nanostructures. Here we present results from extremely high quality 1D hole quantum wires that show up to 10 clean and stable quantized conductance plateaus at B=0 [1,2]. The strong spin-orbit coupling leads to an extreme anisotropy of the Zeeman spin splitting of the 1D hole levels depending on whether the magnetic field is parallel or perpendicular to the quantum wire. Our results show that confining holes to a 1D system fundamentally alters their spin properties, and that it is possible to tune these properties by electrostatically changing the width of the 1D system [3]. [1] O. Klochan, et al, Appl. Phys. Lett. 89, 092105 (2006). [2] R. Danneau, et al, Appl. Phys. Lett. 88, 012107 (2006) [3] R. Danneau, et al, Phys. Rev. Lett., 97 026403 (2006).

10:24AM A44.00011 Quantum dots in graphene. PETER SILVESTROV, K.B. EFETOV, Ruhr-Universitat Bochum — We suggest a way of confining quasiparticles by an external potential in a small region of a graphene strip. Transversal electron motion plays a crucial role in this confinement. Properties of thus obtained graphene quantum dots are investigated theoretically for different types of the boundary conditions at the edges of the strip. The (quasi)bound states exist in all systems considered. At the same time, the dependence of the conductance on the gate voltage carries an information about the shape of the edges.

10:36AM A44.00012 Microwave Conductivity of Silicon Nanowire Arrays. MARK LEE, C. HIGHSTRETE, Sandia National Laboratories*, A.L. VALLETT, S.M. DILTS, J.M. REDWING, T.S. MAYER, The Pennsylvania State University — We have measured the microwave conductivity spectra of silicon nanowire (SiNW) parallel arrays from room temperature to 4K. Doped (n-type and p-type) and nominally undoped SiNWs were synthesized by vapor-liquid-solid growth and assembled by AC dielectrophoresis into parallel arrays spanning the electrodes of coplanar waveguides (CPWs). The CPW complex reflection and transmission coefficients were measured from 0.1 to 50 GHz. Measurements of identical bare CPWs were utilized as a reference for the SiNWs array. We find that the conductivity of the undoped SiNWs is purely imaginary, indicating a bound charge response. The doped SiNWs have a real component that, upon preliminary analysis, increases with frequency consistent with free charge disorder effects. No loss is measured for the undoped SiNWs, but loss due to the doped SiNWs is consistently measured and increases with frequency. *Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
The NMR/NQR spectra of In and Co indicate the presence of electronic inhomogeneity, and the spin-lattice relaxation rate through the State of Texas. Variation of the order parameter becomes essentially one dimensional. We will also discuss the effects of impurities on the quasi-particle density of states.

two-dimensional lattice like. When the impurity concentration reaches certain level, nodal lines of the order parameter no-longer cross each other and the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state at low temperature in d-wave superconductors. At low impurity concentration, the order parameter remains active polymers, colossal magneto resistive systems, nanoscale electronic materials, and Fullerenes, to name a few. Understanding the interplay between strong quantum critical point of this system.

We show that $H_{c1}$ and $H_{c2}$ deduced from Hall probe magnetization and specific heat measurements, respectively are both decreasing with increasing doping content. The corresponding anisotropy parameter $\Gamma_{H_{c2}}(0) = H_{c2}^{ab}(0)/H_{c2}^{c}(0)$ value also decreases from $\sim 5$ in pure MgB$_2$ samples down to $\sim 1.5$ for $x \geq 0.2$ whereas $\Gamma_{H_{c1}}(0) = H_{c1}^{ab}(0)/H_{c1}^{c}(0)$ remains on the order of 1 in all samples. The magnetic field dependence of the anisotropy parameter $\Gamma_{H_{c1}} \leq \Gamma(0) \leq \Gamma_{H_{c2}}$ has then been deduced from a detailed analysis of the angular dependence of the Sommerfeld coefficient for different values of the applied fields. The small and large gap values have been obtained both by fitting the temperature dependence of the zero field electronic contribution to the specific heat to the two gap model and by point contact spectroscopy measurements. Both measurements led to very similar values and the evolution of those gaps with Al concentration suggests that both band filling and interband scattering effects are present.

This work has been performed in collaboration with: L.Lyard, C.Marcenat, J.Marcus, Z.Holanova, P.Szabo, P.Samuely, W.B.Kang, H-J.Kim, H-S.Lee, H-K.Lee, S-I.Lee, S.Tajima and S.Lee.

De Haas-van Alphen Effect across the CeRhIn$_5$ phase diagram.

SWEK K. GOH, University of Cambridge, JOHNPIERRE PAGLIONE, University of California, San Diego, M. SUTHERLAND, C. BERGMANN, University of Cambridge, T. A. SAYLES, M. B. MAPLE, University of California, San Diego — We present de Haas-van Alphen (dHvA) data across the phase diagram of CeRh$_{1-x}$Co$_x$In$_5$ down to ultra-low temperatures. The chemical substitution of Co for Rh, which changes the electronic structure of CeRhIn$_5$, from a localized 4f electron configuration at $x = 0$ to itinerant behaviour at $x = 1$, is analogous to the application of external pressure to the antiferromagnet CeRhIn$_5$, which was shown to exhibit a discontinuous evolution of its Fermi surfaces near 2.35GPa [Shishido et al. J Phys. Soc. Jpn. 74, 1103 (2005)]. Exploiting the rotational degree of freedom afforded by ambient pressure measurements of single-crystal specimens, we analyze both the Fermi surface geometry and quasiparticle effective masses of CeRh$_{1-x}$Co$_x$In$_5$ as a function of chemical substitution in order to investigate the evolution of electronic structure through the antiferromagnetic quantum critical point of this system.

The corresponding anisotropy parameter $\Gamma(0) = H_{c1}^{ab}(0)/H_{c1}^{c}(0)$ and $H_{c2}^{c}(0)$ value also decreases from $\sim 5$ in pure MgB$_2$ samples down to $\sim 1.5$ for $x \geq 0.2$ whereas $\Gamma_{H_{c1}}(0) = H_{c1}^{ab}(0)/H_{c1}^{c}(0)$ remains on the order of 1 in all samples. The magnetic field dependence of the anisotropy parameter $\Gamma_{H_{c1}} \leq \Gamma(0) \leq \Gamma_{H_{c2}}$ has then been deduced from a detailed analysis of the angular dependence of the Sommerfeld coefficient for different values of the applied fields. The small and large gap values have been obtained both by fitting the temperature dependence of the zero field electronic contribution to the specific heat to the two gap model and by point contact spectroscopy measurements. Both measurements led to very similar values and the evolution of those gaps with Al concentration suggests that both band filling and interband scattering effects are present.

This work has been performed in collaboration with: L.Lyard, C.Marcenat, J.Marcus, Z.Holanova, P.Szabo, P.Samuely, W.B.Kang, H-J.Kim, H-S.Lee, H-K.Lee, S-I.Lee, S.Tajima and S.Lee.

Supported by the Material Sciences and Engineering Division Program of the DOE Office of Science under contract DE-AC05-00OR22725 with UT-Battelle, LLC.
12:39PM B8.00006 Fermi-liquid effects in the Fulde-Ferrell-Larkin-Ovchinnikov state of two-dimensional d-wave superconductors, MATTHIAS J. GRAF, Los Alamos National Laboratory, ANTON B. VORONTSOV, Louisiana State University. — We study the effects of Fermi-liquid interactions on quasi-two-dimensional d-wave superconductors in a magnetic field. The phase diagram of the superconducting state, including the periodic Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state in high magnetic fields, is discussed for different strengths of quasiparticle many-body interactions within Landau’s theory of Fermi liquids. Decreasing the Fermi-liquid parameter $F_{DL}$ causes the magnetic spin susceptibility to increase, which in turn leads to a reduction of the FFLO phase. It is shown that a negative $F_{DL}$ results in a first-order phase transition from the normal to the uniform superconducting state in a finite temperature interval. Finally, we discuss the thermodynamic implications of a first-order phase transition for the heavy-fermion superconductor CeCoIn$_5$.

12:51PM B8.00007 Evolution of FFLO state of CeCo(1-x)Cd$_x$. YOSHIFUMI TOKIWA, FILIP RONNING, JOE THOMPSON, ROMAN MOYSOVICH, Los Alamos National Laboratory, LONG PHAM, University of California, Davis, ZACHARY FISK, University of California, Irvine. — Unconventional superconductor CeCoIn$_5$ at high magnetic field displays first order superconducting transition and an additional high field-low temperature superconducting phase (previously proposed to be an inhomogeneous superconducting FFLO state). Both phenomena were attributed to strong Pauli limiting effects. Our specific heat measurements on low Cd-doping (for In) samples, at fields close to the superconducting critical field $H_{c2}$, show that superconducting transition remains first order for samples with $H_{c2}$ up to 5.7 T (from 4.95 T in a pure compound), for field out of plane orientation ($H \parallel c$). We discuss systematic evolution of the proposed FFLO state with Cd content.

1:03PM B8.00008 Specific Heat of Na$_{0.35}$CoO$_2$·1.3H$_2$O: Effects of Sample Age; Two Energy Gaps; Non-Magnetic Pair Breaking, N.E. PHILLIPS, R.A. FISHER, N. OESCHLER, LBNL and University of California, Berkeley, R.J. CAVA, M.-L. FOO, Princeton University, J.E. GORDON, Amherst College — Specific-heat measurements on three samples of Na$_{0.35}$CoO$_2$·1.3H$_2$O show an evolution of the superconductivity and its eventual disappearance with increasing sample age. The results, in combination with other recent work [1], provide a basis for understanding the extreme “sample dependence” of the properties of this material. Samples of different age are in effect samples of slightly different materials. A non-magnetic pair-breaking action produces a residual density of electron states that increases with sample age. It occurs preferentially in the electron band (one of two with different energy gaps) with the smaller gap, producing a change in the nature of the superconducting condensation. It also weakens the overall electron pairing of the superconducting state until it gives way to a competing ordering, possibly a CDW. The same combinations of features in the specific heat have been seen in measurements on other individual samples, showing that they are “intrinsic”. The changes in the specific heat are evidently related to structural and electronic changes that occur on a similar time scale [1], and include an increasing concentration of O vacancies, which could be the pair-breaking scattering centers.

1:15PM B8.00009 Systematic ARPES study on high Na-level Na$_{x}$CoO$_2$ ($x>0.75$), Y.M. XU, Z.H. PAN, P. RICHARD, Boston College, R. JIN, B.C. SALES, D. MANDRUS, Oak Ridge National Laboratory, F.C. CHOU, Massachusetts Institute of Technology, Z. WANG, H. DINING, Boston College. — The phase diagram of the cobaltae Na$_{x}$CoO$_2$, with varying Na concentration x, is very rich and complicated. At the high-doping regime ($x>0.75$), the system was found to be more correlated, with a spin-density-wave state emerging at low temperatures. A previous ARPES study has observed a usually large Fermi surface which apparently violates the Luttinger theorem at $x = 0.8$. We will report our recent ARPES results of the high Na-level Na$_{x}$CoO$_2$ ($x>0.75$) samples.

1:27PM B8.00010 Complete d-Band Dispersion Relation in Sodium Cobaltate, DONG QIAN, L. WRAY, D. HSIEH, L. VICIU, R.J. CAVA, Princeton University, J.L. LUO, D. WU, N.L. WANG, Institute of Physics, Chinese Academy of Sciences, M.Z. HASAN, Princeton University. — We utilize fine-tuned polarization selection coupled with excitation-energy variation of photoelectron signal to image the complete d-band dispersion relation in sodium cobaltates. A hybridization gap anticrossing is observed along the Brillouin zone corner and the full quasiparticle band is found to emerge as a many-body entity lacking a pure orbital polarization. At low dopings, the quasiparticle bandwidth (Fermion scale, many-body EF ~ 0.25 eV) is found to be smaller than most known oxide metals. The low-lying density of states is found to be in agreement with bulk-sensitive thermodynamic measurements for nonmagnetic doping regimes where the 2D Luttinger theorem is also observed to be satisfied.

1:39PM B8.00011 Angle-resolved photoemission study of superconducting cobalt oxide Na$_{1-x}$Co$_2$ yH$_2$O. TAKAIHRO SHIMOJIMA, KYOKO ISHIZAKA, SYUNTARO WATANABE, SHIK SHIN, Institute for Solid State Physics, University of Tokyo, TAKAYUKI KISS, TADASHI TOGASHI, The Institute of Physical and Chemical Research, TAKAYOSHI YOKOYA. The graduate school of Natural Science and Technology, Okayama University, PETRE BADICA, KAZUYOSHI YAMADA, Institute for Materials Research, Tohoku University, KAZUMASA TOGANO, National Institute for Materials Science, Tsukuba, Japan. — Superconducting cobalt oxide Na$_{1-x}$Co$_2$ yH$_2$O is studied by angle-resolved photoemission spectroscopy. We report the Fermi surface topology and electronic structure near the Fermi level in the normal state of Na$_{1-x}$Co$_2$ yH$_2$O. Our result indicates the presence of the hexagonal Fermi surface centered at $\Gamma$ point, while the small pocket Fermi surfaces along 1'-K direction are absent, similar to Na$_2$Co$_2$. The top of the $e'_2$ band, which is expected in band calculations to form the small pocket FSs, extends to within ~30 meV below Fermi level, more closer to Fermi level than in Na$_2$Co$_2$. Its possible role in superconductivity will be discussed, comparing with other experimental and theoretical results.

1:51PM B8.00012 Phase Diagrams, Thermodynamic Quantities and Possible Two Different Superconducting States of Multiorbital Superconductor Na$_x$CoO$_2$·yH$_2$O, MASAHI TOCHIZUKU, RIKEN (The Institute of Physical and Chemical Research); Tokura Multiferroics Project, ERATO, JST, MASAO OGATA, Dept. of Physics, University of Tokyo. — Motivated by recently reported experimental phase diagrams, we theoretically study the effect of Co$_{O_2}$ distortion on the electronic structure in Na$_x$CoO$_2$·yH$_2$O by constructing the multiorbital model. By analyzing the model, we show the deformation of band dispersions and Fermi-surface (FS) topology caused by the variation of Co$_{O_2}$-layer thickness. We propose that two different pairing states, an extended $s$-wave and a $p$-wave pairing, are possible depending on the layer thickness or the FS topology. Furthermore, microscopic calculations of thermodynamic quantities show that two different specific-heat data and two distinct superfluid- density data can be explained fairly well for these two pairing states. We also discuss that inconsistent and scattered experimental results on the magnetic properties, which have been reported from NMR/NQR, $\mu$SR and neutron-scattering measurements, can also be clarified well if we consider the strong layer-thickness dependence.
The pairing mechanism of a hydrated cobaltate superconductor \( \text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O} \) has been of great interest recently. Some experiments point toward unconventional pairing, while others suggest s-wave-like pairing. Recently, based on a fluctuation exchange study for an extended Hubbard model, we have proposed a possibility of unconventional s-wave pairing, where the nesting between the outer and the inner Fermi surfaces that arise due to the local minimum structure of the band at the \( \Gamma \) point plays an important role. The superconducting gap changes sign between the inner and outer Fermi surfaces due to the repulsive interaction originating from the spin fluctuations at the nesting vector, while the gap does not change sign within each Fermi surface. We have further found that this nesting becomes three dimensional when a small hopping integral in the \( z \)-direction is considered, which gives rise to an in-plane ferromagnetic, out-of-plane antiferromagnetic spin correlation, consistent with the experiments for the non-hydrated Na-rich systems. The calculated magnetic ordering temperature and the spin wave dispersion explain well the experimental results.

Monday, March 5, 2007 11:15AM - 2:03PM —
Session B10 DMP: Non-Fermi Liquids Colorado Convention Center Korbel 1E

11:15AM B10.00001 Nonanalytic Magnetic Response of Fermi- and non-Fermi Liquids

Andrey Chubukov, University of Wisconsin, Dmitrii Maslov, Ronojoy Saha, University of Florida — We revisit the issue of the non-analytic dependence of the static spin susceptibility of a 2D Fermi liquid on temperature and a magnetic field, \( \chi_s(T, H) = \chi_0 + AT \chi_s(H) / T \). We show that in a generic Fermi liquid the prefactor \( A \) is expressed via complex combinations of the Landau parameters, and does not reduce to the backscattering amplitude, contrary to the case of the specific heat \( C(T, H) \). We show that this distinction with the specific heat is mostly relevant near a ferromagnetic QCP — the non-analytic terms in \( \chi_s(T, H) \) are less singular near QCP than those in \( C(T, H) \).

11:27AM B10.00002 Derivation of the Marginal Fermi Liquid for the Cuprates

Vivek Aji, Chandra Varma, UC Riverside — The statistical mechanics of the time-reversal and inversion symmetry breaking order parameter, possibly observed in the pseudogap region of the phase diagram of the Cuprates, can be represented by the Ashkin-Teller model. We add kinetic energy and dissipation to the model for a quantum generalization and show that the correlations are determined by two sets of charges, one interacting locally in time and logarithmically in space and the other locally in space and logarithmically in time. The quantum critical fluctuations are derived and shown to be of the form postulated in 1989 to give the marginal Fermi-liquid properties. The model solved and the methods devised are likely to be of interest also to other quantum phase transitions.

11:39AM B10.00003 Pomeranchuk instabilities of Fermi fluids in the spin channel

Kai Sun, U. of Illinois, Congjun Wu, U. of Chicago, Edwardo Fradkin, UUIC, Shou-Cheng Zhang, Stanford — We study the Pomeranchuk instabilities of the Fermi surface in the spin channel. It is shown that the instabilities will lead to two classes of the ordered phases, the \( \alpha \) and \( \beta \)-phases, named by analogy to the superfluid \( ^3\text{He} \)-A and B-phases. The Fermi surfaces in the \( \alpha \)-phases exhibit spontaneous anisotropic distortions, while those in the \( \beta \)-phases remain circular with non-trivial spin configurations in momentum space. The low energy excitations of the ordered phases are studied by RPA approximation. In the \( \alpha \)-phases, the density excitations exhibit anisotropic overdamping and the spin density excitations are nearly isotropic and underdamped at small propagating wavevectors. The \( \beta \)-phases show a Lifshitz-like instability in the \( p \)-wave channel, and will stabilize a chiral ground state inhomogeneity.

11:51AM B10.00004 Theory of non-fermi liquid in a diagonal electronic nematic state

Hae Young Kee, University of Toronto, Ying-Jer Kao, National Taiwan University — We study the fluctuation effects of the diagonal electronic nematic order on a two dimensional square lattice. It has been shown that there exists a quantum critical point between the diagonal nematic and isotropic phases [1]. We study the correlations near the critical point, where the singular forward scattering leads to a non-Fermi liquid behavior over the whole Fermi surface except along the \( (0, \pi) \) and \( (\pi, 0) \) directions. We will also discuss the decay rate of the single-particle excitations as functions of temperature and chemical potential.


12:03PM B10.00005 Diamagnetism of nodal fermions in semimetals: graphene and significant others

Amit Ghosal, Pallab Goswami, Sudip Chakravarty, UCLA — Nodal fermionic excitations are interesting examples of the simplest fermionic quantum criticality in which the dynamic critical exponent \( z = 1 \), and the quasiparticles are well defined. They arise in a number of physical contexts. We derive the scaling form of the diagonal diamagnetism, \( \chi_s \), at finite temperatures, \( T \), and finite chemical potential, \( \mu \). From measurements in graphene, or in \( \text{Bi}_1-x\text{Sb}_x \) \( (x = 0.4) \), one may be able to infer the striking quantum critical Landau diamagnetic susceptibility of the system at \( T = 0 \) and \( \mu = 0 \), \( \chi_s \propto -H^{-1/2} \), \( H \) is the magnetic field. Although the quasiparticles in the mean field description of the proposed \( d \)-density wave (DDW) condensate in a high temperature superconductor is another example of nodal quasiparticles, the crossover from the high temperature behavior, \( \chi_s \propto -T^{-1} \), and the quantum critical behavior of vortex core at a far lower temperature due to the reduction of the velocity scale from the fermi velocity \( v_F \) in graphene to \( \sqrt{\text{FFDDW}} \), where \( v_{\text{DDW}} \) is the velocity in the direction orthogonal to the nodal direction at the Fermi point of the spectra of the DDW condensate.

[1] Supported by NSF-DMR.

12:15PM B10.00006 Self-energy corrections to anisotropic Fermi surfaces

Rafael Roldan, M. Pilar Lopez-Sancho, Francisco Guinea, Instituto de Ciencia de Materiales de Madrid, Shangwen Tsaï, University of California Riverside — The electron-electron interactions affect the low-energy excitations of an electronic system and induce deformations of the Fermi surface. These effects are especially important in anisotropic materials with strong correlations, such as copper oxides superconductors or ruthenates. In this talk I will analyze the deformations produced by electronic correlations in the Fermi surface of anisotropic two-dimensional systems, treating the regular and singular regions of the Fermi surface on the same footing. Simple analytical expressions are obtained for the corrections, based on local features of the Fermi surface, as the Fermi velocity and curvature. It will be shown that, even for weak local interactions, the behavior of the self-energy is non trivial, showing a momentum dependence and a self-consistent interplay with the Fermi surface topology. Applications of the method to cuprates- and \( \text{Sr}_2\text{RuO}_4 \)-like Fermi surfaces will be shown. R. Roldan, M.P. Lopez-Sancho, F. Guinea and S.-W. Tsaï; cond-mat/0003673
12:27PM B10.00007 Gradient Expansion approach to interacting Fermi Liquids, RYUICHI SHINDOU, LEON BAILENTS, Physics Department, University of California, Santa Barbara — Starting from the Keldysh equation for a general multiple band Fermi liquid (FL), we project out fully occupied / empty bands and derive the SU(2) reduced Keldysh equation (RKE), only to discuss the low-energy property of those quasi-particles which are constrained within a single Fermi surface. The RKE thus derived characterizes quasi-particle dynamics in terms of Berry’s curvatures defined in the (d+1) dual space. Namely, in addition to the well-studied “k-space magnetic field”, our Fermi liquid formulations naturally introduce “k-space electric field”, as the Berry’s curvature in frequency and momentum space. When solving the derived RKE in favor of spectral functions, we observe that these artificial electromagnetic fields enter into the linear response of the spectral weight against real applied electromagnetic fields. This theoretical observation naturally lets us raise several photoemission experiments as the candidate experimental tool to measure both U(1) and SU(2) artificial fields in a momentum resolved way, which is widely demanded from the (spin) galvanomagnetic community. Restricting ourselves to the U(1) FLs, we further derive the U(1) Boltzmann equation out of this RKE, to find that not only the artificial magnetic field but also the electric fields enter into the effective EOM for quasi-particles as the Lorentz force in k-space.

12:39PM B10.00008 Effect of Nonmagnetic Impurity in Nearly Antiferromagnetic Fermi Liquid: Magnetic Correlations and Transport Phenomena, HIROSHI KONTANI, MASANORI OHNO, Nagoya University, Japan — In nearly AF metals such as high-Tc superconductors (HTSCs), heavy fermion systems and organic superconductors, a single nonmagnetic impurity frequently causes nontrivial widespread change of the electronic states. To elucidate this long-standing issue, we study a Hubbard model with a strong onsite impurity potential based on an improved fluctuation-exchange (FLEX) approximation, which we call the G_1^{\nu=1/2} FLEX method. We find that (i) both local and staggered susceptibilities are strongly enhanced around the impurity. By this reason, (ii) the quasiparticle lifetime as well as the local DOS are strongly suppressed in a wide area around the impurity (like a Swiss cheese hole), which causes the “huge residual resistivity” beyond the s-wave unitary scattering limit. We stress that the excess quasi-particle damping rate caused by impurities has strong momentum-dependence due to non-s-wave scatterings induced by many-body effects, so that the structure of the “hot spot/cold spot” in the host system persists against impurity doping. This result could be examined by the ARPES measurements. In addition, (iii) only a few percent of impurities can causes a “Kondo-like” upturn of resistivity (\partial p/\partial T < 0) at low temperatures when the system is very close to the AF quantum critical point (QCP). We also discuss the impurity effect in the superconducting state.

12:51PM B10.00009 Kondo physics in a dissipative environment, K. INGERSENT, M. T. GLOSSOP, U. Florida, N. KHOSHKHOU, Wesleyan U. — In recent years impurity models with quantum critical points have attracted much interest. Well-studied examples include the pseudogap and Bose-Fermi Kondo models. In the former model, the depletion of the host density of states at the Fermi level can destroy the Kondo effect; in the latter case, Kondo screening competes with coupling to a dissipative bosonic bath representing, e.g., collective spin fluctuations of the host. The physics of both models is dominated by an interacting quantum critical point. Here, we focus on the more general case of a magnetic impurity interacting with a pseudogap fermionic density of states \rho(\epsilon) \propto |\epsilon|^\nu and with a bosonic bath having a spectral function B(\omega) \propto \omega^\nu. Perturbative renormalization-group (RG) studies of the resulting model, discussed in relation to Kondo temperature suppression in underdoped cuprates [1], have established a rich phase diagram with three stable and two critical fixed points. We report nonperturbative results for this model, obtained using a Bose-Fermi numerical RG approach [2]. We discuss the phase diagram for the Ising-anisotropic case, together with quantum critical properties probed via response to a local magnetic field. [1] M. Vojta and M. Kirčan, PRL 90, 157203 (2003). [2] M. T. Glossop and K. Ingersent, PRL 95, 067202 (2005); PRB (2006).

1Supported by NSF Grant DMR-0312939

1:03PM B10.00010 Nonequilibrium steady-state density of states for a strongly correlated electron system in the presence of a large electric field, ALEXANDER JOURA, JIM FREERRICKS, Georgetown University — The electronic density of states (DOS) of the Falicov-Kimball model in a constant uniform electric field E is calculated using a Kadanoff-Baym-Keldysh nonequilibrium Green’s function technique and dynamical mean-field theory. When the electron-electron interaction U vanishes, the DOS is the Wannier-Stark ladder of delta functions spaced by the Bloch frequency. If U is increased, the delta function peaks initially broaden due to the scattering, but ultimately evolve into a continuous structure for large U. As E is increased from small values, where linear response theory can be used and we see broadened Wannier-Stark peaks, the DOS develops a shape with large peaks at miniband edges, separated in energy by U. We verify the accuracy of our calculations by checking the DOS against frequency-moment sum rules, and an independent transient-response calculation of the Green’s functions at long times. While our formalism has been applied to the Falicov-Kimball model, it can also be directly extended to other models like the Hubbard or periodic Anderson model, by using more complicated impurity problem solvers.

3Work is supported by NSF DMR-0210717

1:15PM B10.00011 Experimental Evidence of Spin-Incoherent Luttinger Liquid State in Semiconductor Quantum wires, MUSTAFA MUHAMMAD, University of Cincinnati, Cincinnati, Ohio 45221, STEVEN HERBERT, Xavier University, Cincinnati, Ohio 45207, RICHARD NEWROCK, PHILIPPE DEBRAY, University of Cincinnati, Cincinnati, Ohio 45221 — We have measured the Coulomb drag between two spatially separated parallel quantum wires in the absence of tunneling to experimentally probe the recently proposed spin-incoherent Luttinger liquid (SILL) state. This new state is considered to exist in one-dimensional electron systems when the electron density is sufficiently low and the electron-electron interaction is strong, leading to J << T << E_F, where J is the exchange coupling of spins and E_F the Fermi energy. The measured drag resistance in the strictly one-dimensional (1D) transport regime is found to follow a power-law temperature dependence with a negative exponent (-0.65) in the temperature range 70mK – 1.2K, in excellent agreement with the prediction of SILL theory for 4k_F. As E is increased from small values, where linear response theory can be used and we see broadened Wannier-Stark peaks, the DOS develops a shape with large peaks at miniband edges, separated in energy by U. We verify the accuracy of our calculations by checking the DOS against frequency-moment sum rules, and an independent transient-response calculation of the Green’s functions at long times. While our formalism has been applied to the Falicov-Kimball model, it can also be directly extended to other models like the Hubbard or periodic Anderson model, by using more complicated impurity problem solvers.

3Work is supported by NSF DMR-0210717

1:27PM B10.00012 Hall effect in strongly correlated low dimensional systems, GLADYS LEON, CHRISTOPHE BERTHOD, THIERRY CIMARCHI, University of Geneva — We investigate the Hall effect in a quasi one-dimensional system made of weakly coupled Luttinger liquids at half filling. A memory function approach is used to compute the Hall resistivity (R_{xy}) in the presence of umklapp scattering along the chains. In this approximation, the Hall resistivity decomposes into two terms linear in the magnetic field: an infinite frequency limit term and a memory term. We investigate the case of zero umklapp scattering, where the memory function vanishes and the Hall resistivity is given by a simple formula corresponding to non-interacting fermions, in agreement with former results made with weakly coupled Luttinger Liquids in the absence of dissipation along the chains. With umklapp scattering present, we find a negative power-law correction to the free-fermion value (band value), with an exponent depending on the Luttinger parameter K_F. We also calculate R_{xy} for the case of noninteracting fermions with umklapp scattering present using Feynman diagrams to compare with the limit K_F → 0 of the power-law result. At high enough temperature or frequency, the Hall coefficient approaches the band value R_{xy} \propto cotan(m\omega T) cond-mat/0608427

This work is supported by the National Science Foundation under grant DMR-0244489
Physics Dept. — We use the two-step density-matrix renormalization group method to extract the critical exponents \( \beta \) of the crystal theory with two copies of chiral multiplets. Exact values of scaling dimensions can be obtained due to the emergent superconformal symmetry although the critical theory becomes the 2+1 dimensional N=2 Wess-Zumino model.

Kavli Institute for Theoretical Physics — We present a two dimensional lattice model which exhibits an emergent space-time supersymmetry at a critical point. The lattice model consists of spinless fermion on the honeycomb lattice and boson on the triangular lattice which is dual to the honeycomb lattice.

Leiden University, Leiden, The Netherlands — The natural spin 1 excitations of 2+1 D antiferromagnets with local interactions, mean field calculations indicate that the amplitudes are generically powerlaw in the bond length with \( \nu \) = 2. Furthermore, the amplitudes are computed from the magnetic side of the transition is \( \beta \) = 1. We find that the exponent \( \beta \) computed from the magnetic side of the transition is consistent with that of the classical Heisenberg model, but not the exponent \( z \nu \) computed from the disordered side. We also show the contrast between integer and half-integer spin cases.

1:39PM B10.00013 Phase space transforms and nonlinear evolution in quantum fluids, RAZVAN TEDOORESCU, Los Alamos National Laboratory — The complex physics of quantum low-dimensional fluids presents challenges that require new theoretical tools and perspectives. In particular, deriving non-linear effective theories that describe strongly interacting, dispersive, one and two-dimensional electrons, is important both for the study of cold fermionic gases and for quasi-one dimensional quantum transport. In this talk, I will present a formalism which reveals connections between the coherent states representation for such systems and non-linear evolution equations obeyed by collective modes. A few applications are also indicated.

1:51PM B10.00014 ABSTRACT WITHDRAWN —

Monday, March 5, 2007 11:15AM - 1:51PM —

Session B11 DMP: Exotic Quantum Phases and Transitions Colorado Convention Center Korbel 1F

11:15AM B11.00001 Spinon Deconfinement at the Quantum Critical Point of 2+1 D Antiferromagnets, ZAIRA NAZARIO, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, DAVID I. SANTIAGO, Instituut-Lorentz, Leiden University, Leiden, The Netherlands — The natural spin 1 excitations of 2+1 D antiferromagnets are made of constituent confined quarks of spin 1/2, spinons. The quantum paramagnetic phase possesses quantum tunneling events or instantons, which confine the spinons. There have been recent suggestions of new critical points where spinons are deconfined. Instanton events which cause the spinon confinement disappear at the deconfined critical point because the massless spinons screen them effectively and because instanton tunneling becomes infinitely costly. We point out that this happens irrespective of the intrinsic spin of the antiferromagnet. Hence spinons are deconfined irrespective of microscopic spin. Berry phase terms relevant to the paramagnetic phase make the confinement length scale diverge more strongly for half-integer spins, next strongest for odd integer spins, and weakest for even integer spins. There is an emergent photon at the deconfined critical point, but the ‘semimetalllic’ nature of critical spinons screens such photon making it irrelevant to long distance physics.

11:27AM B11.00002 Experimental Consequences of O(3) Deconfined Criticality in 2+1 D Antiferromagnets, DAVID I. SANTIAGO, Instituut-Lorentz, Leiden University, ZAIRA NAZARIO, Max Planck Institute for the Physics of Complex Systems, Dresden — The paramagnetic phase of 2+1 D antiferromagnets can be described in terms of electrodynamics of charged, massive bosonic spinons interacting through an emergent compact U(1) gauge field. Spinons in the paramagnet are confined due to the presence of nontrivial tunneling effects, instantons which provide a long range interaction between the gauge fields and the charges that gaps the gauge fields and provides a linear potential for the charges. The instantons responsible for spinon confinement in the paramagnetic phase vanish at the quantum critical point. Therefore, spinons are deconfined at criticality. We have recently obtained the effective theory that describes the universal physics of these deconfined critical points. From the deconfined critical theory, we calculate the critical Neel field propagator and find a critical exponent \( \eta = 1 \). We also obtain measurable effects and quantities that follow from the prediction \( \eta = 1 \) and serve as characterization of O(3) deconfined criticality. Those are the inelastic and elastic neutron scattering response, Nuclear Magnetic Resonance (NMR) response, magnetic field response and the specific heat. All of these response functions serve to define the O(3) deconfined universality class.

11:39AM B11.00003 Emergent supersymmetry at a critical point of a lattice model, SUNG-SIK LEE, Kavli Institute for Theoretical Physics — We present a two dimensional lattice model which exhibits an emergent space-time supersymmetry at a critical point. The lattice model consists of spinless fermion on the honeycomb lattice and boson on the triangular lattice which is dual to the honeycomb lattice. It will be shown that there is only one relevant perturbation at the supersymmetric critical point and the critical theory becomes the 2+1 dimensional \( N = 2 \) Wess-Zumino theory with two copies of chiral multiplets. Exact values of scaling dimensions can be obtained due to the emergent superconformal symmetry although the critical theory is the interacting theory.

11:51AM B11.00004 Critical exponents in a transition between an AFM and a valence bond crystal, SAMUEL MOUKOURI, University of Michigan, Physics Dept. and Center for Theoretical Physics, KENNETH GRAHAM, University of Michigan, Physics Dept. — We use the two-step density-matrix renormalization group method to extract the critical exponents \( \beta \) and \( \nu \) in the transition from a Néel phase to a magnetically disordered phase with a spin gap. We find that the exponent \( \beta \) computed from the magnetic side of the transition is consistent with that of the classical Heisenberg model, but not the exponent \( z \nu \) computed from the disordered side. We also show the contrast between integer and half-integer spin cases.

12:03PM B11.00005 Self-optimized resonating-valence-bond trial wavefunctions, KEVIN BEACH, ANDERS SANDVIK, Boston University — The spin singlet ground state of a quantum antiferromagnet can be expanded in the overcomplete basis of valence bond states. [1] To first approximation, the weight associated with each configuration is factorizable into a product of individual bond amplitudes. For nonfrustrated antiferromagnets with local interactions, mean field calculations indicate that the amplitudes are generically powerlaw in the bond length with exponent \( d - 1 \), where \( d \) is the dimension of the lattice. Such states can be employed as the initial trial state for a valence bond projector calculation of the exact ground state. [2] Moreover, the amplitudes can be determined self-consistently by measuring the statistics of the bonds appear in the projected state and feeding this information back into the trial state. It is also possible to build some of the neglected bond-bond correlations into the trial state itself. The next level of approximation is to factorize the weights in terms of amplitudes that depend on the lengths and orientations of two valence bonds. Again, these amplitudes can be self-optimized in a simulation by matching them to the bond-bond correlations of the projected state.


1Supported by grant NSF DMR-0513930.
12:15PM B11.00006 Simulating finite-momentum states of quantum spin systems in the valence bond basis\(^1\), ANDERS SANDVICK, KEVIN BEACH, Boston University — Quantum spin systems such as the Heisenberg model can be simulated numerically in the valence bond basis, as an alternative to the standard basis of eigenstates of the \(S_z\) operators \([1]\). One advantage of this approach is that also the triplet sector can be studied based on the configurations generated in the singlet sector \([1,2]\). This way an improved estimator for the singlet-triplet gap can be constructed. Here we show that also finite-momentum triplet states can be studied [in practice for \(q \ll 0\) or \(\pi \ll q\) due to a phase problem], thus allowing us to calculate the triplet dispersion \(E(q)\). Matrix elements \(\langle T(q)|S_z^2|0\rangle\) are also accessible. These matrix elements give directly the magnon weight in the dynamic structure factor \(S(q,\omega)\). We also discuss how deconfined spinon excitations can be detected in this approach.

\(^1\)Supported by the NSF under grant No. DMR-0513930.

12:27PM B11.00007 Spin-liquid phase in a spin-1/2 quantum magnet on the kagome lattice, SERGEI ISAKOV, YONG BAEK KIM, ARUN PARAMEKANTI, University of Toronto — We study a model of hard-core bosons with short-range repulsive interactions at half filling on the kagome lattice. This model is equivalent to an easy-axis spin-1/2 quantum model with no special conservation laws. Using quantum Monte Carlo methods we numerically study the ground state. We find a instability at half-filling. The bosonic version of this model has been recently studied and found to have several unusual features. Fermionic models tend to be more tractable. We also identified a large class of fluctuationless states specific to the fermionic models — a result hinting at a possible explanation of the extended possibility of a new charge ordered liquid phase.

12:39PM B11.00008 First-order phase transition in a gauge theory of \(S = 1/2\) quantum antiferromagnets in the deep easy-plane limit\(^1\), ASLE SUDBO, STEINAR KRAGSET, EIVIND SMORGRAV, JOAKIM HOVE, Norwegian University of Science and Technology, FLAVIO NOGUEIRA, Freie Universit"{a}t Berlin — We perform large-scale Monte Carlo simulations on an effective gauge theory for a spin-1/2 easy-plane antiferromagnet, including a Berry phase term that projects out the \(S = 1/2\) sector. Without a Berry phase term, the model exhibits a phase transition in the 3DXY\(^1\) universality class associated with proliferation of gauge-charge neutral U(1) vortices. The instantons that eliminate the phase transition in the gauge-charged sector are suppressed by the Berry phases. The result is a first-order phase transition.

\(^1\)Work supported by the Norwegian Research Council.

12:51PM B11.00009 Non-Abelian Anyon Superconductivity, WAHEB BISHARA, Caltech, CHETAN NAYAK, Microsoft Station Q and UCLA — Non-Abelian Anyons are proposed to exist in certain spin models and in Quantum Hall systems at certain filling fractions. In this work we studied the ground state of dynamical SU(2) level \(\kappa\) Chern Simons non-abelian anyons at finite density and no external magnetic field. We find that in the large \(\kappa\) limit the topological interaction induces a pairing instability and the ground state is a superconductor with \(d + id\) gap symmetry. We also develop a picture of pairing for the special value \(\kappa = 2\) and argue that the ground state is a superfluid of pairs for all values of \(\kappa\).

1:03PM B11.00010 Strongly correlated fermions on frustrated lattices, FRANK POLLMANN, Max Planck Institute for the Physics of Complex Systems, KIRILL SHTENGEL, UC Riverside, JOSEPH BETOURAS, SUPA, University of St. Andrews, ERICH RUNGE, TU Ilmenau, PETER FULDE, Max Planck Institute for the Physics of Complex Systems — Systems with frustrated interactions are generally characterized by a high density of low-lying excitations which leads to a high susceptibility and thus interesting physical effects. We study a novel class of strongly correlated fermions on frustrated lattices which allows for excitations which carry fractional charges \([1]\). For a systematic study, we firstly consider a model of spinless fermions on a geometrically frustrated planar pyrochlore (checkerboard) lattice. An effective Hamiltonian is derived for the strongly correlated limit which describes the low-lying excitations. We solve the fermionic sign problem for the latter Hamiltonian and thus make it possible to apply quantum Monte Carlo methods \([3]\). The ground state is shown to be charged ordered and fractional charges are linearly confined. Secondly, we consider a model of spinful fermions on the kagome lattice and study the interplay between charge – and spin – degrees of freedom. \([4]\) P. Fulde, K. Penc, and N. Shannon, Annalen der Physik 11, 892 (2002) \([2]\) E. Runge and P. Fulde, Phys. Rev. B 70, 245113 (2004) \([3]\) F. Pollmann, J. J. Betouras, K. Shtengel, and P. Fulde, Phys. Rev. Lett. 97, 170407 (2006)

1:15PM B11.00011 Spinless Fermions on a Checkerboard Lattice, KIRILL SHTENGEL, UC Riverside, FRANK POLLMANN, Max Planck Institute for the Physics of Complex Systems, JOSEPH BETOURAS, SUPA, University of St. Andrews, PETER FULDE, Max Planck Institute for the Physics of Complex Systems — We present a study of the low-energy physics of a spinless fermionic model on a checkerboard lattice at half-filling. The bosonic version of this model has been recently studied and found to have several unusual features. Fermionic models tend to be more interesting: the inherent sign problem resulting from the fermionic statistics makes them notoriously difficult to handle. The low-energy physics of the model can be described by a fermionic quantum loop model on the square lattice. We found a non-localization that can, in certain cases, cure the sign problem. We also identified a large class of fluctuationless states specific to the fermionic models — a result hinting at a possible explanation of the extended ground-state entropy recently found in a few other fermionic models. Finally, we looked at the so-called Rokhsar-Kivelson quantum critical point, where we found the exact ground state(s) as well as studied the low-lying excitations. This allowed us to make several educated guesses about the phase diagram for the model in question. \([1]\) F. Pollmann, J. J. Betouras, K. Shtengel, and P. Fulde, Phys. Rev. Lett. 97, 170407 (2006)

1:27PM B11.00012 Spinless charges on the triangular lattices in the strong repulsion limit: possibility of a new charge ordered liquid, NOBUO FURUKAWA, CHISA HOTTA, Dept. Physics, Aoyama Gakuin Univ. — We propose a new type of charge ordered liquid state in the spinless fermion system on a triangular lattice under strong inter-site Coulomb interactions, \(V\). In the absence of fermion hoppings, the ground state is disordered due to geometrical frustration. Introduction of hopping terms lifts the degeneracy and drives the system to a metallic state with possible partial charge orderings, which we call a “pinball liquid”. There, a gapless charge liquid component moves around a possible long range ordered Wigner crystal component. This liquid state is dominant over wide range of filling, \(n = 1/3 \sim 2/3\). When an anisotropy in \(V\) exceeds its critical value at half-filling \(n = 1/2\), an metal-insulator transition accompanied by another charge order with a different periodicity is induced. Relevance to the organic conductors \(\theta\)-ET\(_2\)X which show novel nonlinear transport properties is discussed.

REFERENCES: cond-mat/0605045, cond-mat/0607181, cond-mat/0607717.

1:39PM B11.00013 Local density of states in electronic nematic phase, HYEONJIN DOH, HAE-YOUNG KEE, University of Toronto — We study spatial patterns of local density of states in electronic nematic phase in the presence of a non-magnetic impurity. Since the Fourier transform of the spatial pattern represents the symmetry of an electronic structure of a system, the local density of state can be a direct probe for the isotropic-nematic phase transition. In this work, we show local density of states near the nematic-isotropic phase transition tuned by a magnetic field, and discuss its application to the bilayer ruthenate, \(\text{Sr}_2\text{Ru}_2\text{O}_7\).
Monday, March 5, 2007 11:15AM - 2:15PM –
Session B12 GMAG DMP FIAP: Focus Session: Spin Injection

11:15AM B12.00001 Highly Efficient Room Temperature Spin Injection Using Spin Filtering in MgO
, XIN JIANG, IBM Almaden Research Center, San Jose, CA 95120 — Efficient electrical spin injection into GaAs/AlGaAs quantum well structures was demonstrated using CoFe/MgO tunnel spin injectors at room temperature. The spin polarization of the injected electron current was inferred from the circular polarization of electroluminescence from the quantum well. Polarization values as high as 57% at 100 K and 47% at 290 K were obtained in a perpendicular magnetic field of 5 Tesla. The interface between the tunnel spin injector and the GaAs interface remained stable even after thermal annealing at 400 °C. The temperature dependence of the electron-hole recombination time and the electron spin relaxation time in the quantum well was measured using time-resolved optical techniques. By taking into account of these properties of the quantum well, the intrinsic spin injection efficiency can be deduced. We conclude that the efficiency of spin injection from a CoFe/MgO spin injector is nearly independent of temperature and, moreover, is highly efficient with an efficiency of ~ 70% for the temperature range studied (10 K to room temperature). Tunnel spin injectors are thus highly promising components of future semiconductor spintronic devices.

Collaborators: Roger Wang1,3, Gian Salis2, Robert Shelby1, Roger Macfarlane1, Seth Bank3, Glenn Solomon3, James Harris3, Stuart S. P. Parkin1
1 IBM Almaden Research Center, San Jose, CA 95120
2 IBM Zurich Research Laboratory, Säumerstrasse 4, 8803 Rüschlikon, Switzerland
3 Solid States and Photonics Laboratory, Stanford University, Stanford, CA 94305

11:51AM B12.00002 Electrical spin injection from Fe into AlxGa1−xAs quantum well spin-LEDs
1, IMRAN KHAN, MANUEL DIAZ-AVILA, MESUT YASAR, ATHOS PETROU, SUNY at Buffalo, AUBREY T. HANBICKI, GEORGE KIOSEOGLOU, BEREND T. JONKER, Naval Research Laboratory — We have studied Fe spin LEDs in which electron-hole recombination takes place either in GaAs or in AlxGa1−xAs quantum wells (QW). The dependence of the electroluminescence circular polarization P on temperature T in these two types of devices at fixed magnetic field is compared. The polarization in the AlxGa1−xAs QW LEDS decreases much more slowly with temperature compared with the GaAs QW LEDs; the polarization of the former persists up to room temperature. The improved high temperature performance of the AlxGa1−xAs spin LEDs is tentatively attributed to the localization of the recombining electron-hole pairs by potential fluctuations in the QW. These sites have zero-dimensional character suppressing the Dyakonov-Perel spin scattering mechanism.

1 Work at SUNY was supported by ONR (N000140610174) and NSF (ECS0524403).

12:03PM B12.00003 Spin injection from Fe into GaAs quantum wells populated by electrons or holes: A comparison
1, A. PETROU, M. YASAR, I. KHAN, M. DIAZ-AVILA, SUNY AT Buffalo, G. KIOSEOGLOU, A.T. HANBICKI, B.T. JONKER, Naval Research Laboratory — We have studied the circular polarization of band-edge electroluminescence (EL) from three types of AlxGa(n)/GaAs(i)/AlxGaAs(p) light emitting diodes (LEDs) in which the electrons are injected from ferromagnetic Fe contacts. In the first (second) group the GaAs quantum well is populated by electrons (holes) due to excess n-type (p-type) doping in the n-AlGaAs (p-AlGaAs) barrier. In the third device type the GaAs quantum wells are empty and these LEDs are used as reference samples. We have compared the magneto-optical characteristics (dependence of the EL circular polarization P as function of magnetic field, current, and photon energy) of these three groups. Significant differences have been identified which must be taken into account in order to determine accurately the spin injection efficiency of these devices.

1 Work at SUNY was supported by ONR (N000140610174) and NSF (ECS0524403).

12:15PM B12.00004 Generation and detection of spin current in GaAs with MgO tunnel barriers Replace
, Y.J. PARK, Francis Bitter Mag. Lab., MIT, Cambridge, MA 02139 / Nanodevice Res. Center, Korea Inst. of Sci. and Tech., Seoul, Korea, M. VAN VEENHUIZEN, J.S. MOODERA, Francis Bitter Mag. Lab., MIT, Cambridge, MA 02139, C.H. PERRY, D. HEIMAN, Dept. of Phys., Northeastern Univ., Boston, MA 02115 — The MgO tunnel barrier has been proven as one of best candidates for the spintronic memory and switching devices. When one injects and detects spin polarized carriers efficiently into (and out of) semiconductors, the use of tunnel barrier (TB) is expected to avoid the conductivity mismatch and provide a high feasibility for the fabrication of a spin transistor. To reach this goal evaluation of the TB on a semiconductor is an important issue. In this work, we report the combination of spin dependent photocurrent generation and electrical detection as an efficient technique for understanding the role of the MgO TB grown on GaAs. We used (100)GaAs/MgO/Fe structures prepared in an MBE chamber. Our results show that spin filtering effects are largely influenced by the quality of MgO TBs. The estimated photocurrent polarization reaches up to approximately 80% at RT in a certain forward bias region which is associated with transport processes. The efficient room temperature spin filtering for GaAs/MgO/Fe structures observed here has not been reported yet for either Fe/GaAs or Fe/AlxOy/GaAs structure. The possible origin will be discussed in detail.

12:27PM B12.00005 Electrical spin injection from Fe1−xGa x (001) films into AlGaAs/GaAs(001) LEDs
1, G. KIOSEOGLOU, A.T. HANBICKI, O.M.J. VAN ’T ERVE, C.H. LI, M. OSOFSKY, S.-F. CHENG, B.T. JONKER, Naval Research Laboratory — Electron spin polarizations of 40-70% have been obtained in GaAs due to electrical injection from Fe or FeCo contacts using surface-emitting spin-LEDs. In such LEDs, since Fe has its magnetization easy axis in the substrate plane, a large magnetic field (>2.2 tesla) along the surface normal is required to saturate the magnetization out-of-plane. We have grown epitaxial films of Fe1−xGa x (0 < x < 0.75), a material noted for its high magnetostriiction, on AlGaAs/GaAs (001) heterostructures, and summarize the structure, magnetization, spin polarization, and results for electrical spin injection into AlGaAs/GaAs. The out-of-plane saturation field and magnetization decrease rapidly with Ga content, but the point contact spin polarization remains near that of Fe for x < 0.5. Electrical spin injection from an Fe0.5Ga0.5 contact produces an electron spin polarization of 30% in the GaAs at 20 K, similar to that obtained from Fe contacts, but with out-of-plane saturation fields as low as 0.4 T. Post-annealing at low temperature increases the electron spin polarization up to 40% and it will be discussed at the meeting.

1 This work was supported by ONR.

The high momentum electrons are promoted to the higher energy L and X valleys by the strong electric field at the Fe/semiconductor interface.

1 Work at SUNY was supported by ONR (N000140610174) and NSF (ECS0524403).

12:39PM B12.00006 Electron distribution among the \( \Gamma, L, \) and \( X \) GaAs conduction band valleys in an Fe/GaAs(n) Schottky barrier.

1 Work at SUNY was supported by ONR (N000140610174) and NSF (ECS0524403).

12:51PM B12.00007 Electrical spin injection into the ground and excited states of uniform InAs quantum dots.

1 Work at SUNY was supported by ONR (N000140610174) and NSF (ECS0524403).

1:03PM B12.00008 Measurement of the spin detection efficiency of the s, p, d, and f shells in InAs QDs using optical pumping.

1 Work at SUNY was supported by ONR (N000140610174) and NSF (ECS0524403).

1:15PM B12.00009 Model for the Bias Dependence of the Sign of Spin Injection in Ferromagnetic Metal/Semiconductor Schottky Tunnel Contacts.

1 Supported by ONR and DARPA/MTO.

1:27PM B12.00010 Hot electron injection, vertical transport, and electrical spin detection in Silicon.

1 Supported by ONR and DARPA/MTO.

12:39PM B12.00011 All Epitaxial Heterostructure for Spin Injection from a Half Metal into Silicon.

1 Supported by ONR and DARPA/MTO.
1:51PM B12.00012 Non-equilibrium Fe-Si thin films as potential spin injection materials. JIAN ZHOU, ERIK HELGREN. University of California at Berkeley, LI ZENG, UCSD, FRANCES HELLMAN, University of California at Berkeley — Fe-Si thin films are potential spintronics materials for its tunable structural, magnetic, and electric properties [1]. Our goal is to inject spin polarized electrons from iron-silicides into Si through a Schottky barrier, which is formed by choosing the proper doping level for Si, and a suitable iron-silicide composition. We prepared Fe$_{1-x}$Si$_x$ (x = 0.25 - 0.5) films by electron beam co-evaporation from Fe and Si sources onto Si substrates under ultra-high vacuum conditions. Growth at 300 °C leads to a homogenous Fe$_{1-x}$Si$_x$ magnetic alloy with both Tc and room temperature magnetization monotonically decrease with an increasing x. X-ray diffraction patterns show that a thinned layer of Fe$_{1-x}$Si$_x$ at interface reduces the lattice mismatch between Si substrate and the bcc Fe$_{1-x}$Si$_x$ film, so that epitaxial growth can be realized. The seed layer also plays the role of reducing interdiffusion. A clear interface at iron-silicide and silicon is obtained, resulting in a good Schottky barrier with height around 0.7 eV. By adjusting the Fe$_{1-x}$Si$_x$ composition, the resistivity of iron-silicide can be tailored. Ferromagnetic Fe$_{0.75}$Si$_{0.25}$ shows resistivity of 10$^{-3}$ ohm-cm, and magnetization 100 emu/cc at 300 K. By increasing the iron-silicide resistivity, one of the main obstacles for spin-injection from metal to semiconductor — the resistivity mismatch — can be overcome. Experiments based on spin-valve-type magneto-resistance for spin injection detection will be discussed. [1] Ionescu et al. Physical Review B 71, 94401 (2005).

2:03PM B12.00013 Spin Injection and Spin Dynamics at CuPc/GaAs (100) Interface. HOA SHA, SHUAN JING, University of Maryland, College Park, MARINA SANCHEZ-AlBANEDA, MRKO CINCHETTI, JIAN-PETER WUSTENBERG, OLEKSYI ANDREYEV, MICHAEL BAUER, MARTIN AESCHLIMANN, Department of Physics, University of Kaiserslautern — Spin injection from CuPc (100) to organic semiconductor copper phthalocyanine (CuPc) has been investigated experimentally with spin-resolved two-photon photoemission (SR-2PPE) spectroscopy. The spin-polarized electrons are originally generated in GaAs through optical pumping with femtosecond time resolution and injected into CuPc film. We observed an enhancement in spin polarization at the interface after initial CuPc deposition. This demonstrates that interface spin scattering is insignificant, which is similar to our previous results of spin injection at CuPc/Co interface. The spin polarization dropped when the CuPc film became thick, an effect attributed to bulk attenuation in CuPc. The lifetime of the unoccupied orbits in CuPc was also studied with red-blue excitation of photon energy of 1.6 eV and 3.2 eV, respectively. There was a strong asymmetry in the time-resolved spectra, and an unexpected long lifetime for the low intermediate state was observed. A simple explanation of this phenomenon will be discussed.

---

Monday, March 5, 2007 11:15AM - 2:15PM — Session B13 DMP GMAG: Focus Session: Cobaltates and Manganites Colorado Convention Center Korbel 4C

11:15AM B12.00001 Tuning Physical Properties via Isovalent Doping in Ba$_{2-x}$Sr$_x$CoO$_4$. HAO SHA, JIAN DI ZHANG, Department of Physics, Florida International University, Miami, FL 33199, Q. HUANG, NIST Center for Neutron Research, Gaithersburg, Maryland 20899, V.O. GARLEA, B.C. SALES, M. ANDREAS, R. JIN, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — It is known that monoclinic Ba$_2$CoO$_4$ is an antiferromagnetic (AFM) insulator with Neel temperature $T_N=25$K. We found that isovalent Sr substitution for Ba drastically changes the structural and magnetic properties of Ba$_{2-x}$Sr$_x$CoO$_4$ system. With increasing x, $T_N$ initially increases then decreases after reaching the maximum at x=0.5. Correspondingly, its crystal structure changes from monoclinic (x $< 0.5$) to orthorhombic (x $> 0.5$) at room temperature. The correlation between structure and physical properties will be discussed.

11:27AM B12.00002 Spin-state transitions and magnetic polaron in lightly doped La$_{1-x}$Sr$_x$CoO$_3$. A. PODLENSKY, Hahn-Meitner-Institut, Berlin, Germany, M.W. HAVERKORT, II Physikalisches Institut, Universitaet zu Koeln, Germany, K. CONDER, Paul Scherrer Institut, Villigen, Switzerland, E. POMYAKUSHINA, ETH Zurich & Paul Scherrer Institute; Villingen, Switzerland, DANIEL KOHMSKI, II Physikalisches Institut, Universitaet zu Koeln, Germany — Using the inelastic neutron scattering (INS) technique, we identified the energy levels of the thermally excited states of Co$^{3+}$ ions in both La$_2$CoO$_3$ and La$_{0.988}$Sr$_{0.012}$CoO$_3$. In La$_{0.988}$Sr$_{0.012}$CoO$_3$ an excitation at $\sim$0.6 meV appears at T $> 30$K, whose intensity follows the bulk magnetization. Within a model including crystal field interaction and spin-orbit coupling we interpret this excitation as originating from a transition between thermally excited states located about 120 K above the ground state. Since the g-factor obtained from the field dependence of the INS is g $> 3$, we interpret this state as a high-spin state of Co$^{3+}$. The lightly doped material x=0.002 exhibits paramagnetic properties at low temperatures. An INS peak at energy transfer $\sim$0.75 meV was observed in it already at $T = 1.5$ K. We propose that the holes introduced in the LS state of La$_2$CoO$_3$ by doping are extended over the neighboring Co sites, forming thus magnetic polaron and transforming all the involved Co ions (e.g. 6 of them) to the high-spin state. Similarly to LaCoO$_3$, we interpret the INS transition at 0.75 meV as that on these high-spin Co$^{3+}$ ions.

11:39AM B12.00003 Incommensurate Spin Correlations in La$_{1-x}$Sr$_x$CoO$_3$. D. PHELAN, D. LOUCA, K. KAMAZAWA, S.-H. LEE, University of Virginia, S. ROSENKRANZ, J.F. MITCHELL, S.N. ANCONA, MSD, Argonne Natl Lab, M.F. HUNDLEY, Los Alamos Natl Lab, Y. MOTOMO, University of Tokyo, Y. MORITOMO, University of Tsukuba — Non-magnetic, insulating La$_2$CoO$_3$ is transformed into a metallic, spin cluster ferromagnet when holes are added to the system by replacing La$^{3+}$ with Sr$^{3+}$. Previous work has shown that this transition results from the percolation of isotropic, ferromagnetic clusters. Here, we present elastic neutron scattering data which shows that a short-ranged, anisotropic incommensurate magnetic phase also appears as holes are added. We have studied this incommensurate phase in detail for a number of concentrations, spanning the phase diagram above and below the percolative phase transition, and the incommensurability increases with the hole concentration. From the evolution of the incommensurate signal strength with x, we concluded that the incommensurate phase is competing with the FM clustering. The spin incommensurability may originate from a local ordering of magneto-polarons.

11:51AM B12.00004 A non-Griffiths-like clustered phase above the Curie temperature of the doped perovskite cobaltite La$_{1-x}$Sr$_x$CoO$_3$. CHUNYONG HE, MARIA TORIJA, JING WU, University of Minnesota, JEFF LYNN, NIST Center for Neutron Research, JOHN MITCHELL, Argonne National Laboratory, CHRIS LEIGHTON, University of Minnesota — The existence of preformed clusters above the Tc of the doped perovskite manganites is well established and, in many cases, conforms to the expectations for a Griffiths phase. We show here that the phase-separated perovskite cobaltite (La$_{1-x}$Sr$_x$CoO$_3$) also exhibits a clustered state above the Tc in the ferromagnetic phase. The formation of magnetic clusters at a well-defined temperature ($T^*$) is revealed in the small-angle neutron scattering, d.c. susceptibility, and resistivity. Remarkably, this clustered state has none of the characteristics of a Griffiths phase; the deviation from Curie-Weiss behavior is opposite to expectations and is not field dependent, and $T^*$ does not correspond to the undiluted Tc. These results demonstrate that although the Griffiths phase may occur in many systems with quenched disorder, it is not universally applicable to the randomly doped transition metal oxides.

---

3 We acknowledge support from DOE (DE-FG02-06ER46275), NSF (DMR-0509666), and the ACS PRF, as well as neutron facilities at NIST. Work at ANL supported by US DoE under W-31-109-ENG-38.
Competing ferromagnetic and incommensurate order in perovskite cobaltites La$_1$-$_x$Sr$_x$CoO$_3$. STEPHAN ROSENKRANZ, Materials Science Division, Argonne National Laboratory — Many phenomena observed in complex oxides, and in particular their enhanced response to external fields, are intimately linked to the existence of short-range order such as formation of stripes, ladders, checkerboards or phase separation. This nanoscale disorder results from the delicate balance of spin, orbital, charge, and strain degrees of freedom that leads to competing groundstates with incompatible order. Inhomogeneity in the form of phase separation is also believed to play a key role in the magnetoresistance of doped cobalt perovskites La$_1$-$_x$Sr$_x$CoO$_3$. In this system, doping holes into the non-magnetic, insulating parent compound leads to spin-glass behavior at low doping, with nanoscale ferromagnetic clusters forming within a non-ferromagnetic matrix. Percolation of these isolated clusters therefore physical properties. Work supported by NSF DMR.

**12:39PM B13.00006 Thickness dependence of the structural, magnetic, and electronic properties of epitaxial La$_{0.5}$Sr$_{0.5}$CoO$_3$ films on SrTiO$_3$(001) substrates**. MANISH SHARMA, MARIA TORIJA, CHRIS LEIGHTON, Department of Chemical Engg. and Material Science, University of Minnesota — Bulk La$_{1-x}$Sr$_x$CoO$_3$ (LSCO) materials have received considerable attention due to the existence of spin-state transitions, magneto-electronic phase separation, and giant anomalous Hall effect. In our prior work we have established optimized conditions for the deposition of high quality epitaxial LSCO thin films. In this work, we provide a comprehensive study of the variation of structural, morphological, magnetic, and electronic properties as a function of film thickness. This investigation has been carried out as a controlled function of oxygen stoichiometry using the total sputtering pressure (30, 70, and 140 mTorr, at an O$_2$ / Ar ratio of 0.4) as the control parameter. High resolution WAXRD, x-ray rocking curves, x-ray reflectivity, AFM, d.c. magnetometry, and electronic transport measurements have all been employed. Our results indicate that the thickness dependence of the electronic and magnetic properties is dominated by the sensitive interplay between oxygen stoichiometry and strain relaxation. The behavior at very low thickness is discussed in terms of the known phenomenology of the magneto electronic phase separation in this material.

**12:51PM B13.00007 Fabrication, characterization, and magnetic and electronic properties of epitaxial La$_{0.5}$Sr$_{0.5}$CoO$_3$ films**. M.A. TORIJA, M. SHARMA, J. WU, C. LEIGHTON, University of Minnesota — Bulk La$_{1-x}$Sr$_x$CoO$_3$ (LSCO) has received considerable attention with regard to magnetic phase separation. Fabrication of epitaxial films would provide a means to study this phase separation under dimensional confinement. We have investigated the properties of epitaxial films of x = 0.5 LSCO on SrTiO$_3$ (001) by reactive d.c. sputtering from compound targets. Structure and properties were studied as a function of sputtering pressure, O$_2$/Ar ratio, and post-deposition O$_2$ treatment. Optimized conditions result in single phase, stoichiometric, substantially relaxed, epitaxial films. At a fixed O$_2$ / Ar ratio, two distinct regimes of total sputtering pressure (P) occur. Films grown at P > 50 mTorr have properties close to bulk; they are ferromagnetic (T$_C$ ≈ 230 K, $M_S$ ≈ 2 $\mu_B$/Co), have a metallic-like $\rho$(T) at all T, and exhibit 10% magnetoresistance at T$_C$. For P < 50 mTorr, we obtain lower surface roughness and narrower rocking curves but with low moment, insulating $\rho$(T), and increased out-of-plane lattice parameter due to O deficiency. Similarly, a dramatic enhancement in physical properties, and elimination of a CoO minority phase, is obtained when cooling in 500 Torr of O$_2$. The results demonstrate good control over the oxygen stoichiometry, and therefore physical properties. Work supported by NSF DMR.

**1:03PM B13.00008 Doping Dependence of Polaron Hopping Energies in La$_{1-x}$Ca$_x$MnO$_3$ (0 ≤ x ≤ 0.15)**. KRISHNA NEUPANE, JOSHUA COHN, University of Miami, JOHN NEUMEIER, Montana State University — Measurements of the low-frequency ($f < 100$ kHz) permittivity at T ≤ 160 K and dc resistivity (T ≤ 430 K) are reported for La$_{1-x}$Ca$_x$MnO$_3$ (0 ≤ x ≤ 0.15). Static dielectric constants are determined from the low-T limiting behavior of the permittivity. The estimated polarizability for bound holes $\sim 10^{-22}$ cm$^3$ implies a radius comparable to the interatomic spacing, consistent with the small polaron picture established from prior transport studies near room temperature and above on nearby compositions. Relaxation peaks in the dielectric loss associated with charge-carrier hopping yield activation energies in good agreement with low-T hopping energies determined from variable-range hopping fits of the dc resistivity. The doping dependence of these energies suggests that the orthorhombic, canted antiferromagnetic ground state tends toward an insulator-metal transition that is not realized due to the formation of the ferromagnetic insulating state near Mn$^{4+}$ concentration $\sim 0.13$.

**1:15PM B13.00009 Magnetic susceptibility of La$_{0.7}$Ca$_{0.3}$MnO$_3$ at very low magnetic fields in the vicinity of the ferromagnetic transition**. JOHN J. NEUMEIER, JOSE A. SOUZA, Montana State University, YI-KUO YU — Magnetic susceptibility ($\chi$) measured at magnetic fields $H$ as low as 0.2 Oe is reported for La$_{0.7}$Ca$_{0.3}$MnO$_3$. A pronounced enhancement in $\chi$ is observed in the region above the critical temperature $T_c$, at very low $H$. As the magnetic field is increased, this feature is shifted toward $T_c$, eventually vanishing near $H = 400$ Oe. Electrical resistivity measurements show a positive magnetoresistance effect between 0 and 500 Oe in a temperature range slightly above $T_c$. The results are discussed in a scenario of frustrated magnetism and the possibility of a Griffiths singularity is addressed. This material is based upon work supported by NSF (DMR-0504769 and 0552458) and the Brazilian agency CNPq (201017/2005-9).
2:03PM B13.00013 Structural and magnetic properties of SrMn$_{1-x}$Ru$_x$O$_3$ perovskites. B. DABROWSKI, S. KOLESNIK, O. CHMAISSEM, T. MAXWELL, Department of Physics, Northern Illinois University, DeKalb, IL. -- Ferromagnetism of SrRuO$_3$ is unique among 4d transition metal based perovskite oxides. On substitution of Mn its $T_C$ decreases from 163 K to 0 for $x$ = 0.5-0.6 followed by a formation of an antiferromagnetic insulating state at a quantum critical point. The other end member of the SrMn$_{1-x}$Ru$_x$O$_3$ family, a cubic perovskite SrMnO$_3$ is a G-type antiferromagnet with $T_C$=233 K. We have synthesized the complete SrMn$_{1-x}$Ru$_x$O$_3$ solid solution. The polycrystalline samples were characterized by neutron diffraction, magnetic, and transport experiments. The incorporation of Ru in the SrMnO$_3$ matrix (0.1<x<0.4) results in a phase transition to a C-type antiferromagnetic state accompanied by a cubic-tetragonal transition. The intermediate substitution level induces a spin-glass behavior, due to competing ferro- and antiferromagnetic interactions. Mixed valence Mn$^{3+}$/Mn$^{4+}$ and Ru$^{4+}$/Ru$^{3+}$ pairs introduce additional frustration to the magnetic states. The glassy behavior can be observed for $x$ up to 0.7 in the tetragonal structure. Supported by NSF (DMR-0302617) and the U.S. Department of Education

Deceased
12:03PM B14.00003 Magnetic Stripe Domains in Thermally Evaporated Ni Strips. SOO HYUNG LEE, FRANK ZHU, CHIA-LING CHIEN, NIINA MARKOVIC, Johns Hopkins University — We have studied thermally evaporated thin Ni strips with varying widths and geometries. Magnetic force microscopy images showed the presence of magnetic stripe domains. Wide Ni strips in their as-prepared-state exhibited stripe domains oriented perpendicular to the edge of the samples. In contrast, narrow Ni strips showed stripe domains that were parallel to the edge. Changes to the geometry of the strips caused competition of different stripe orientations. After we demagnetized the strips with an in-plane field, stripe domains followed the field’s direction, which was at an arbitrary angle to the edge of the sample. We will discuss these results in terms of existing theoretical models.

12:15PM B14.00004 Oscillatory Curie Temperature of Fe/ Cu-wedge/ Fe/ Cu(111) nanodots. NOPPI WIDJAJA, Univ of Tennessee and ORNL, W.C. LIN, National Taiwan University, K. FUCHIGAMI, Univ of Tennessee, ORNL and IHI, M.A. TORIJA, Univ of Tennessee, M.-T. LIN, National Taiwan University, E.W. PLUMMER, Univ of Tennessee and ORNL. J. SHEN, ORNL and Univ of Tennessee — The interactions between two layers of Fe nanodots were studied as a function of the thickness of a Cu spacer layer. The bottom Fe-dot layer was grown on a Cu(111) substrate cleaned in situ by cycles of Ne-ion sputtering and annealing, employing a magnet gas buffer layer assisted growth (BLAG) technique. Subsequently, a wedge-shaped Cu spacer layer was evaporated to cap the Fe-dots, followed by the growth of the top Fe-dot layer using the same BLAG method. Wedge-shaped samples are crucial for this study because the effects we are looking for are often subtle and would have been obscured by fluctuations in preparation conditions if we had to prepare a separate sample for each thickness. In-situ magneto-optical Kerr effect (MOKE) measurements were utilized to determine the local Curie temperature (T_C) at various positions on the wedged samples, and regular oscillations in T_C as a function of the spacer layer thickness were observed.

1Work supported by DOE Division of Materials Sciences and Engineering under contract DE-AC05-00OR22725, and by NSF under Contract No. DMR 0451163.

12:27PM B14.00005 Temperature dependence of the uncompensated magnetization in Fe_{Ni_{1−x}}Fe_{x}/Co bilayers. DAVID LEDERMAN, MIYEON CHEON, ZHONGYUAN LIU, Department of Physics, West Virginia University — A giant uncompensated magnetization in Fe_{Ni_{1−x}}Fe_{x}/Co was observed in the hysteresis loops at low temperatures (T < T_{B} ~ 55 K), whose sign was correlated with the sign of theexchange bias field H_{EB}. In this study, the uncompensated magnetization of x = 0.05, 0.21 and 0.49 samples was studied at different temperatures. The uncompensated magnetization was reversed at H = −16 kOe (H = −14 kOe) going from positive to negative fields and H = +14 kOe (H = +11 kOe) going from negative to positive fields at T = 30 K for the x = 0.05 (x = 0.21) sample. This asymmetry in the reversal means that the uncompensated magnetization in these samples has its own exchange bias field of H_{EB} ~ −1 kOe with a coercivity of 14 kOe. In the case of the x = 0.49 sample, the uncompensated magnetization has a coercivity of 23 kOe and a positive exchange bias H_{EB} = +10 kOe at T = 30 K. The coercive fields of the uncompensated magnetization decrease as the temperature increases while the magnitude of the uncompensated magnetization remains constant.

1This work was supported by the National Science Foundation.
2Presently at State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, China

12:39PM B14.00006 Magnetic properties of one dimensional Ni/ Cu (Al) /Ni nanowires: Role of non-magnetic spacer. PARTHA PRATIM PAL, RANJIT PATI, Department of Physics, Michigan Technological University — One dimensional (1-D) magnetic multilayered nanowires with alternating ferromagnetic and non-magnetic structures arranged in sequence have been the subject of intense research in recent years for their potential applications in magneto-electronics or spintronics. We have used first-principles periodic density functional theory to study the stability, electronic, and magnetic properties of Ni/Cu/ Ni and Ni/Al/ Ni nanowires. The thickness of the non-magnetic spacer layer is systematically changed to explore the role of non-magnetic spacer in controlling the interlayer magnetic coupling and hence the magnetic properties of these 1-D nanowires.

12:51PM B14.00007 Dipole-Exchange modes in ferromagnetic nano-wires of arbitrary cross sections. RODRIGO ARIAS, Universidad de Chile, DOUGLAS MILLS, UC Irvine — We present a method that allows to calculate the eigen- frequencies of dipole-exchange modes in ferromagnetic nano- wires of arbitrary cross sections. The method is setup for calculating modes of long wavelength along the main direction of the nano-wire, but it could be extended to short wavelengths. The basis of the theoretical approach is the extinction theorem, under a form appropriate for the inclusion of the exchange interaction. Appropriate integral equations in the form of contour integrals around the periphery of the wire are obtained for the mostof the target properties and magnetization of the modes. We perform a numerical analysis of the eigen- frequencies of geometries of interest, like rectangular and elliptical cross sections, recovering the appropriate limiting values of the magnetostatic or exchange dominated regimes.

1This research has been supported by the U. S. Army, through Contract No. CS0001028, and R. A. has received support also from FONDECYT(Chile), Grant No. 1061106.

1:03PM B14.00008 High Magnetization FeCo/Pd multilayers. MICHAEL WALOCK, MINT Center, The University of Alabama, FRANK KLOSE, The Spallation Neutron Source, Oak Ridge National Laboratory, MAIRBEK CHSHIEV, GARY MANKEY, WILLIAM BUTLER, MINT Center, The University of Alabama — A high saturation magnetization is advantageous in magnetic recording. Currently, the peak of the Slater-Pauling curve is the BCC FeCo system with a saturation magnetization of 2.45 T. Recently, a magnetization of 2.57 T in the FeCo layers of a [40 nm Fe_{30}Co_{70}/1.7 nm Pd]_{25} superlattice has been reported [1, 2]. This behavior may be attributed to an enhanced Fe moment in the expanded FCC matrix, and an accompanying induced moment in the Pd. Our experimental results show an intrinsic moment enhancement, but this is not great enough to overcome the overall magnetization density reduction caused by the incorporation of Pd in the matrix. The overall effect is a reduced magnetization. Through variation of the FeCo composition and Pd layer thickness, and the combinatorial methods of structural and magnetic characterization, we will gain insight into the magnetic structure of this tertiary thin film system. [1] K. Noma, M. Matsuoka, H. Kanai, Y. Uehara, K. Nomura, and N. Awaji. IEEE Trans. Magn. 42, 140 (2006). [2] ibid. 41, 2920 (2005).

1This project was funded by grants from the DOE & NSF-DMR 0213985

1:15PM B14.00009 Modulating magnetic properties of the one dimensional (1-D) Fe/Pt /Fe multilayered Nanowires: A first principles study. PUSPAMITRA PANIGRAHI, RANJIT PATI, Department of Physics, Michigan Technological University — Using first-principles density functional theory within the Local Spin Density Approximation (LSDA), we have predicted the stability, electronic and magnetic properties of 1-D ferromagnetic Fe/Pt/Fe multilayered nanowires. The thicknesses of the magnetic and non-magnetic spacer layers are systematically varied to study the evolution of magnetic properties with the spacer size. The stability of the nanowire is found to increase with the increase of the thickness of the Pt layer in the nanowire, we found that the average magnetic moment per Fe atom in the ferromagnetic configuration can be enhanced significantly.
Effects Colorado Convention Center Korbel 4F

We studied the effect of changing the strength of the coupling between the Fe contacts and the fullerene molecule. We find that strong coupling leads to metallic Fe-contact spins. Specifically, the current varies by 15-20% as the orientation of the Gd spin moment is changed with respect to that of Fe contacts. We also functional theory and the Landauer-Buttiker formalism, we demonstrate that the total current depends on the relative orientation of the Gd spin and the two 82

TIMM, University of Kansas, FLORIAN ELSTE, Freie Universitaet Berlin — Electronic transport through magnetic molecules has recently received considerable attention. This is partly motivated by the idea to integrate spintronics with molecular electronics. This talk highlights a number of interesting effects we include fingerprints of magnetic excitations seen in inelastic tunneling beyond the sequential-tunneling approximation, very slow spin relaxation, giant spin 100

TIMM, University of Kansas, FLORIAN ELSTE, Freie Universitaet Berlin — Electronic transport through magnetic molecules has recently received considerable attention. This is partly motivated by the idea to integrate spintronics with molecular electronics. This talk highlights a number of interesting effects we include fingerprints of magnetic excitations seen in inelastic tunneling beyond the sequential-tunneling approximation, very slow spin relaxation, giant spin 74

2:03PM B14.00013 The importance of the dipolar interaction strength in magnetization hysteresis curves of two-dimensional nanomagnet arrays1, RICHARD KLEMM, MARISOL ALCANTARA ORTIGOZA, Kansas State University, TALAT RAHMAN, University of Central Florida — Recently, Takagaki and Ploog [Phys. Rev. B 71, 184439 (2005)] used a fourth-order Runge-Kutta technique to integrate the Landau-Lifschitz-Gilbert equations for square lattices of \( N \times N \) magnetic nanodots with dipolar interdot interactions. Some of their results appeared to differ qualitatively from the second-order Runge-Kutta results obtained for the same systems by Kayali and Saslow [Phys. Rev. B 70, 174404 (2004)], both in the hysteresis area \( A_N \) and in the number of steps of the magnetization hysteresis loops. We [Phys. Rev. B 74 (22), xxxxxx (2006), in press] show that these differences are not due to inaccuracies in either calculation or to the potentially different magnetic induction sweep rates used, but can be attributed entirely to different choices of the dipolar interaction strength \( h_{\text{dip}} \propto a^{-3} \), where \( a \) is the two-dimensional lattice constant. 1Supported in part by the NSF through Contract No. NER-0304665

Monday, March 5, 2007 11:15AM - 2:15PM — Session B16 GMAG DCOMP DMP: Focus Session: Spin Transport and Orbital Polarization Effects Colorado Convention Center Korbel 4F

11:15AM B16.00001 Spin-dependent electronic transport through magnetic molecules1, CARSTEN TIMM, University of Kansas, FLORIAN ELSTE, Freie Universitaet Berlin — Electronic transport through magnetic molecules has recently received considerable attention. This is partly motivated by the idea to integrate spintronics with molecular electronics. This talk highlights a number of interesting effects we predict for tunneling through single magnetic molecules and molecular monolayers weakly coupled to metallic leads. The results are obtained in a rate-equation approach which treats the intra-molecular interactions exactly and works also for situations far from equilibrium (large bias voltage). Effects to be discussed include fingerprints of magnetic excitations seen in inelastic tunneling beyond the sequential-tunneling approximation, very slow spin relaxation, giant spin amplification, and negative differential conductance at high temperatures. 1Supported by the KU Center for Research and the German Science Foundation through Sfb 658

11:27AM B16.00002 Spin-polarized transport through the endohedral fullerene Gd@C_{82}, LAXMIDHAR SENAPATI, STEVEN C. ERWIN, Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375 — We investigate theoretically the spin-polarized electron transport through an endohedral metallofullerene Gd@C_{82} sandwiched between magnetic Fe contacts. Using density-functional theory and the Landau-Buttiker formalism, we demonstrate that the total current depends on the relative orientation of the Gd spin and the two Fe-contact spins. Specifically, the current varies by 15-20% as the orientation of the Gd spin moment is changed with respect to that of Fe contacts. We also studied the effect of changing the strength of the coupling between the Fe contacts and the fullerene molecule. We find that strong coupling leads to metallic current-voltage characteristics, while weak coupling leads to Coulomb blockade.
11:39AM B16.00003 Magnetic phenomena, spin orbit effects, and electron transport in Pt nanowire contacts. ALEXANDER SMOGUNOV, SISSA, Democritos, ICTP, ANDREA DAL CORSO, SISSA, Democritos, EROIS TOSATTI, SISSA, Democritos, ICTP — We present a first-principles DFT study of the electronic, magnetic, and transport properties of short monatomic Pt nanowire contacts. For an infinite tipless Pt wire a fully relativistic calculation, including spin-orbit effects, yields a ferromagnetic ground state already for the unstrained wire [1]. We found that short 3-atom and 5-atom stressed wires in contact with nonmagnetic Pt leads remain locally magnetic, with the magnetization parallel to the wire axis, owing to orbital magnetism. Ballistic conductance of these nanowires is calculated using the scattering-based method [2]. Preliminary results indicate a ballistic conductance for a stressed 5-atom wire of about 2.9 $G_0$ ($G_0 = 2e^2/h$ is the conductance quantum) for parallel magnetization, 2.3 $G_0$ for perpendicular magnetization, and 2.4 $G_0$ in the nonmagnetic case. The former is in closest agreement with experimental values reported in break junctions [3].


11:51AM B16.00004 Progress in ab initio methods for spin transport1, ALEXANDRE ROCHA2, School of Physics, Trinity College Dublin — Numerical simulations have an important role in spintronics, here one envisages the use of the spin as well as the electron charge for electronic applications. In this talk we will present our code Smeagol [1] which combines the non-equilibrium Green function formalism with density functional theory and it has been specifically designed for magnetic devices. With Smeagol we will first investigate the possibility of large ballistic magnetoresistance in nickel point contacts, addressing the effects of local exchange and correlation functionals as well as the possible presence of oxygen impurities. Then I will describe an attempt to integrate the fields of spin- and molecular-electronics by constructing spin-valves using organic molecules. I will demonstrate that it is possible to obtain different transport behaviour, large magnetoresistance [1] as well as current rectification and spin-diode effects by simply selecting the molecule and the anchoring groups. Finally I will show how Smeagol is a valuable tool for simulating spin-polarised STM images.

References


1Supported by: NRI, NSF MRSEC

12:27PM B16.00005 Calculations of spin-disorder resistivity from first principles1, ALEKSANDER WYSOCKI, KIIRILL BELASHCHENKO, JULIAN VELEV, Department of Physics and Astronomy, University of Nebraska Lincoln, MARK VAN SCHILFGAARDE, Department of Chemical and Materials Engineering, Arizona State University — Spin-disorder resistivity of Fe and Ni is studied using the noncollinear density functional theory. The Landauer conductance is averaged over random disorder configurations and fitted to Ohm’s law. The distribution function is approximated by the mean-field theory. The dependence of spin-disorder resistivity on magnetization in Fe is found to be in excellent agreement with the results for the isotropic s-d model. In the fully disordered state, spin-disorder resistivity for Fe is close to experiment, while for fcc Ni it exceeds the experimental value by a factor of 2.3. This result indicates strong magnetic short-range order in Ni at the Curie temperature. We suggest that the analysis of calculated and measured spin-disorder resistivity provides a powerful method to extract information on the temperature dependence of the magnetic short-range order parameter in ferromagnetic metals.

[1] R.T.S. acknowledges financial support from TÜBA-GEBIP

12:39PM B16.00006 Size-dependent alternation of magnetoresistive properties in atomic chains1,2, R. TUGRUL SENGER, ENGIN DURGUN, HALDUN SEVINCI, Bilkent University, HATEM MEHREZ, SALIM CIRACI, Bilkent University — Spin-polarized electronic and transport properties of carbon atomic chains are investigated when they are capped with transition-metal (TM) atoms like Cr or Co, using density functional theory. The magnetic ground state of the TM-C$_n$-TM chains alternates between the ferromagnetic (F) and antiferromagnetic (AF) spin configurations as a function of n. The desirable AF state is obtained for only even-n chains with Cr; conversely only odd-n chains with Co have AF ground states. We present a simple model that can successfully simulate these variations, and the induced magnetic moments on the carbon atoms. Depending on the relative strengths of the spin-dependent couplings and the on-site energies of the TM atoms there induces long-range spin polarizations on the carbon atoms which mediate the exchange interaction. When connected to appropriate electrodes these atomic chains display a strong spin-valve effect. Analysis of electronic and magnetic properties of these atomic chains, and the indirect exchange coupling of the TM atoms through carbon chain will be presented.1 E. Durgun et al., J. Chem. Phys. 125, 121102 (2006).2 E. Durgun et al., Phys. Rev. B 74 (in press).

1R.T.S. acknowledges financial support from TÜBA-GEBIP

12:51PM B16.00007 T-dependent matrix elements in x-ray magnetic circular dichroism, YONGBIN LEE, BRUCE HARMON, ALAN GOLDMAN, Ames Laboratory - US DOE, JONATHAN LANG, Argonne National Laboratory — Dramatic changes in the Er L$_2$ and L$_3$ XMCD spectra in Er$_2$Fe$_{17}$ as a function of temperature have been investigated with detailed experiments and first principles calculations. This study seeks to understand the fundamental mechanisms governing the spectral shape and magnitude of the L$_2$ and L$_3$ XMCD spectra as a step toward developing XMCD as a quantitative probe for rare earths similar to its effectiveness for transition metals via the use of sum rules (which do not work for rare earths). The XMCD spectra as a step toward developing XMCD as a quantitative probe for rare earths similar to its effectiveness for transition metals via the use of sum rules (which do not work for rare earths). The calculations simulate the key thermal physics by evaluating the spin polarized band structures obtained with the 4f moment on the Er atom constrained to values of 0, 1, 2, and 3 Bohr magnetons. Both the theory and our experiments, performed at the Advanced Photon Source, show the XMCD L$_2$-edge spectrum changes sign as the temperature is lowered, and the L$_3$-edge spectrum also shows systematic and significant changes. We will discuss the effects of dipole matrix elements, spin-orbit coupling, hybridization between 5d-3d orbital, and magnetic anisotropy on the XMCD spectra. Quadrupole transitions and core hole effects will also be discussed.

1:03PM B16.00008 Orbital Polarization in Itinerant Magnets, IGOR SOLOVYEV, National Institute for Materials Science, Tsukuba, Japan — The correct description of the orbital magnetism is one of the longstanding problems in the density functional theory (DFT). One possible solution is to extend DFT by considering explicit dependence of the exchange-correlation energy on the orbital degrees of freedom. Since the angular momentum operator does not commute with electrostatic potential, it is not an observable except a small atomic region where this potential is nearly spherical. Hence, the orbital magnetism is an atomic property, and we inevitably have to deal with the problem of on-site Coulomb interactions and screening of these interactions in solids.1 For itinerant systems, this screening can be evaluated in the random-phase approximation (RPA), by considering the strong-coupling electron-electron interactions. In these cases, the ground-state properties are determined by the mean-field theory. The dependence of spin-disorder resistivity on magnetization in Fe is found to be in excellent agreement with the results for the isotropic s-d model. In the fully disordered state, spin-disorder resistivity for Fe is close to experiment, while for fcc Ni it exceeds the experimental value by a factor of 2.3. This result indicates strong magnetic short-range order in Ni at the Curie temperature. We suggest that the analysis of calculated and measured spin-disorder resistivity provides a powerful method to extract information on the temperature dependence of the magnetic short-range order parameter in ferromagnetic metals.


1:15PM B16.00009 Magnetic circular dichroism and the orbital magnetization of ferromagnets, IVO SOUZA, University of California and LBNL, Berkeley, DAVID VANDERBILT, Rutgers University — The spontaneous magnetization of ferromagnets has both spin and orbital contributions, $M = M_{\text{spin}} + M_{\text{orb}}$, which can be separated out via gyromagnetic measurements. Recently, it was found that, when expressed as a bulk property of the Bloch electrons, the orbital magnetization itself consists of two terms, $M_{\text{orb}} = M_{\text{LC}} + M_{\text{IC}}$, which can be loosely interpreted as the localized and itinerant contributions, respectively. Interestingly, $M_{\text{LC}}$ and $M_{\text{IC}}$ are separately gauge-invariant, which raises the possibility that they may be independently measurable. We shall see that indeed they are related to the magnetic circular dichroism (MCD) spectrum by a subtle sum rule. MCD, the difference in absorption between left- and right-circularly-polarized light, is given by $\sigma_{A_{\text{orb}}}^{(2)}(\omega)$, the absorptive part of the antisymmetric conductivity. We derive the following sum rule for the interband contribution: $\int_0^\infty \sigma_{A_{\text{orb}}}^{(2)}(\omega)d\omega = (2\pi e^2/h)\left(M_{\text{LC}} - M_{\text{IC}}\right)$, where $\sigma_{A_{\text{orb}}}^{(2)}(\omega)$ is a pseudo-vector. Hence, by combining the results of gyromagnetic and magneto-optical experiments, $M_{\text{LC}}$ and $M_{\text{IC}}$ in principle be measured independently.

1:27PM B16.00010 Alternative approach to ab-initio NMR spectra for periodic systems, TIMO THONHAUSER, Rutgers University/Massachusetts Institute of Technology, ARASH MUSTOFI, NICOLÀ MARZARI, Massachusetts Institute of Technology, DAVID VANDERBILT, Rutgers University, RAFFAELE RESTA, University of Trieste — We propose a novel finite-differences approach for computing the NMR response in periodic solids that is based on the theory of orbital magnetization recently introduced by some of us. Instead of obtaining the shielding tensor from the response to an external magnetic field, we derive it directly from the orbital magnetization appearing in response to a microscopic magnetic dipole. This procedure has an established parallel in the case of electric fields, where Born effective charges are often obtained from the polarization induced by a sublattice displacement instead of the force induced by an electric field. Among the advantages of the present approach are its simplicity and its applicability to situations in which linear-response theory would be cumbersome.

1:39PM B16.00011 Orbital magnetization in a supercell framework: Single k-point formula, DAVIDE CERESOLI, SISSA and Democritos National Simulation Center, Trieste, RAFFAELE RESTA, University of Trieste and Democritos National Simulation Center, Trieste — The position operator $r$ is ill-defined within periodic boundary conditions: owing to this, both the macroscopic (electric) polarization and the macroscopic orbital magnetization are nontrivial quantities. While the former has been successfully tamed since the early 1990s, the latter remained a long-standing unsolved problem. A successful formula within DFT for crystalline systems has been recently found. The formula is based on a Brillouin-zone integration, which is discretized on a reciprocal-space mesh for numerical implementation. We find here the single k-point limit, useful for large enough supercells, and particularly in the framework of Car-Parrinello simulations for noncrystalline systems. We validate our formula on the test case of a crystalline system, where the supercell is chosen as a large multiple of the elementary cell. Rather counterintuitively, even the Chern number (in 2d) can be evaluated using a single k-point diagonalization.

1:51PM B16.00012 Orbital magnetism of mesoscopic integrable system, MING LOU, SLAVA SEROTA, University of Cincinnati — In the mesoscopic regime, magnetic properties (such as orbital magnetism) are sensitive to whether the corresponding classical dynamics is chaotic or integrable. Non-interacting electron gas in a rectangular box is proposed as a “generic” model to study orbital magnetism of integrable systems. We derived the exact energy level correlation function for this system, including the perturbation by magnetic field. Combining the exact correlation function and Imry’s formalism, we calculated the orbital magnetic susceptibility and discussed the field dependence at $T \rightarrow 0$ and temperature dependence at $B \rightarrow 0$. As a result, the susceptibility $\chi \sim |k_F L| \sqrt{\omega_F} \left\{ \log \left( \phi_0 / \phi \right) \left( T \rightarrow 0, \phi \ll \phi_0 \right) \log \left( \sqrt{\Delta E} / T \right) \left( B \rightarrow 0, T \ll \sqrt{\Delta E} \right) \right\}$, where $k_F L$ is the Landau susceptibility, $k_F$ is the Fermi vector, $L$ is the rectangle’s side, $\phi_0$ is the magnetic flux quantum, $\Delta$ is the mean level spacing, and $E_F$ is the Fermi energy. For high temperature and large field, the mesoscopic part of susceptibility exponentially vanishes and only the bulk Landau diamagnetism is left. The logarithmic divergence at zero field and zero temperature is consistent with previous numerical calculations and is a manifestation of pronounced non-self-averaging properties of integrable systems.

2:03PM B16.00013 Orbital Ordering in Cs$_2$AgF$_4$ - an electronic structure study, DEEPA KASINATHAN, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, KLAUS KOEPERNIK, IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany; Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, ULRIKE NITZSCHE, IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany, HELGE ROSNER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — The argentate Cs$_2$AgF$_4$, first synthesized in 1974 has many similarities to the high-$T_c$ cuprates, featuring AgF$_2$ sheets in place of CuO$_2$ sheets. While the undoped cuprates are antiferromagnetic, this argentate is ferromagnetic with a $T_{\text{Curie}}$ of about 15 K. Density functional calculations in the proposed tetragonal structure produce an itinerant half-metallic ferromagnet. Recent inelastic neutron scattering experiments have suggested an orbital-ordered structure that allows an orbital ordered ferromagnetic ground state. We performed electronic structure calculations using the LDA+U method on this system and were able to obtain an orbitally ordered ground state, not only for the newly proposed orbital lattice but also for the original tetragonal lattice by constraining the bravais lattice and allowing the change of the atomic basis. In specific, very small changes in the position of the in-plane fluorine atoms already trigger an orbital ordering. Our calculated energy scale shows that this orbital ordered state should be stable for all temperatures, consistent with the experiment.

Monday, March 5, 2007 11:15AM - 2:15PM — Session B17 DPOLY DMP: Focus Session: Pentacene and Field Effect Transistors, Colorado Convention Center 102

11:15AM B17.00001 Organic Field Effect Transistors, C. DANIEL FRISBIE, University of Minnesota — This talk will present an introduction to organic field effect transistors (OFETs) including results for pentacene thin film transistors, which have become a benchmark for organic electronics. We will also discuss the use of high capacitance gate dielectrics in OFETs to achieve large two dimensional carrier densities and metallic conductivity in OFETs.
11:51AM B17.00002 Growth of pentacene on inorganic and organic dielectrics and sub-micron channel OTFT fabrication1, G. LEISING, B. STADLOBER, U. HAAS, A. HAASE, H. GOLD, Joanneum Research / Inst. of Nanostructured Materials and Photonics — We have fabricated pentacene thin films on different organic and inorganic dielectrics at four substrate temperatures with different film thicknesses ranging from the submonolayer over the multilayer to the “thick” film regime. These films were characterized by AFM and analyzed by means of scaling and rate equation theory in order to deduce the molecular growth dynamics. We found that on all substrates and in a certain substrate temperature range the growth can be well described as diffusion-limited aggregation. A critical island size was deduced from the scaling of the distribution density of the grain areas and the power-law dependence of the saturated nucleation density on the deposition rate. OTFTs with a channel length down to 300 nanometers have been fabricated by nanoimprint-lithography, using stamps made by e-beam-lithography and reactive ion etching. Due to a combination of different effects these transistors show high quality electrical characteristics. In conclusion, we observed no principal limitation for the downsampling of pentacene-based OTFTs due to short channel effects concerning all relevant parameters such as threshold voltage, mobility, on-current and on-off ratio as long as the morphology is characterized by large and well-ordered crystallites.

1Part of this work was funded by the “POLYAPPLY” integrated EC-project (contract no. 507143).

12:03PM B17.00003 The improvement of out of plane crystalline size of pentacene thin films on plastic substrates by transfer printing1, S.A. SOLIN, Y. SHAO, Washington University in St. Louis, D.R. HINES, E.D. WILLIAMS, University of Maryland — Pentacene thin films on plastic substrates were fabricated using the transfer printing method. [1] The out of plane structural order, structure disorder factor and crystalline size were studied by X-ray diffraction.[2] The effects of transfer printing control parameters, such as temperature and pressure, on the crystalline size and structural disorder were quantified using paracrystal theory. The calculated average number of reflecting net planes in the crystalline domains N and the disorder factor gII agree with the a* law. The 12~16% improvement of out of plane crystalline size was observed for pentacene printed at 100~120 °C. Higher printing pressure 600 PSI improved the crystallinity above that obtained with low pressure 100 PSI. Pentacene printed at 120 °C and 600 PSI showed both optimal growth axis crystalline size of 283 Å and mobility 0.237 cm²/Vs, respectively. The optimized crystalline size shows a direct correlation with the improvement of the carrier mobility of pentacene thin transistors. [1] D. R. Hines et al., Appl. Phys. Lett. 86, 163101 (2005). [2] Y. Shao et al., J. Appl. Phys. 100, 44512 (2006).

1 Supported by the NSF, by the WU CMI, and by the Laboratory for Physical Sciences at UMD.

12:15PM B17.00004 Enantiotropic Polymorphs in Pentacene1, THEO SIEGRIST, Bell Laboratories, Murray Hill, NJ 07974, CELINE BESNARD, EPFL, Lausanne, Switzerland, SIMON HAAS, ETHZ, Zurich, Switzerland, MARK SCHILTZ, PHILIP PATTISON, EPFL, Lausanne, SWITZERLAND, DMITRY CHERNYSHOV, S.NBL, ESRF, Grenoble, France, BERTRAM BATLOGG, ETHZ, Zurich, Switzerland, CHRISTIAN KLOC, Bell Laboratories — The high temperature structural phase transformation in bulk pentacene has been characterized by X-ray single crystal and powder diffraction. A well-defined transition temperature of 463K was observed in single crystals. In contrast, pentacene powders heated above the phase transformation temperature do not always fully convert, and upon cooling, coexistence of the two polymorphs in varying concentrations is observed down to room temperature. The 12° order phase transformation is intracrystalline, whereby the close packed herringbone-type layers shift against each other, keeping the same symmetry. The present results demonstrate that the structure of pentacene first reported in 1961 is actually stable only at high temperatures, and thus metastable at room temperature.

1 Supported in part under DOE contract DE-FG02-04ER46118.

12:27PM B17.00005 Effect of impurities on pentacene thin film growth for field-effect transistors1, ELBA GOMAR-NADAL, BRAD R. CONRAD, ELLEN D. WILLIAMS, Physics Department and Materials Research Science and Engineering Center, University of Maryland, College Park, MD 20742 — The presence of impurities in organic semiconductors is one of the factors that limit device performance. Among all organic semiconductors, pentacene has shown the highest mobility reported to date. The effect of a controlled introduction in pentacene thin films of a well characterized impurity, 6,13-pentacenequinone (PnQ), was investigated. Since the majority of charge carriers in organic field effect transistors (OTFT) are located at the semiconductor-dielectric interface, this work focuses on the correlation between pentacene ultrathin film morphology and the overall OTFT device performance. The introduction of large amounts of PnQ revealed the presence of crystalline domains characteristic of pure PnQ submonolayer growth. The change of crystalline structure of the initial submonolayer for smaller amounts of PnQ is being investigated. The transistor mobility is dramatically reduced by increasing the degree of PnQ in the source material.

1The University of Maryland MRSEC is supported by the National Science Foundation

12:39PM B17.00006 Aggregation of pentacene molecules on SiO2 substrates and its influence on the FET characteristics. GENKI YOSHIKAWA, J. T. SADOWSKI, A. AL-MAHBOOB, Y. FUJIKAWA, T. SAKURAI, IMR, Tohoku University, Y. TSURUMA, S. IKEDA, K. SAIKI, The University of Tokyo — Pentacene is one of the most promising materials for organic field effect transistors (OFETs). In order to improve the FET performance, dielectric layers, such as SiO2, are commonly modified by the self-assembled monolayers (SAMs), such as hexamethyldisilazane (HMDS). Owing to utilization of these SAMs, the performance of the pentacene FET has exceeded that of amorphous Si FET. However, we have found that pentacene molecules deposited on HMDS-treated SiO2 substrates aggregate with time even under ultra-high-vacuum (UHV) and ambient temperature conditions. We constructed an in situ atomic force microscopy (AFM)-FET measurement system and found that the FET mobility significantly decreased with the aggregation. Thus, this aggregation should be one of the major origins of the instability and irreproducibility of pentacene-based devices. In order to reveal the mechanism of the aggregation, we carried out an in situ and real time observation of growth and the aggregation of pentacene molecules on the several substrates, such as clean SiO2 and HMDS, under UHV conditions with low energy electron microscope (LEEM). We have found that pentacene tends to aggregate on the substrate with lower surface energy.

12:51PM B17.00007 Orientation of Pentacene Molecules on SiO2: From a Monolayer to the Bulk. FAN ZHENG, Department of Physics, University of Wisconsin Madison, BYOUNG-NAM PARK, SOONJOO SEO, PAUL G. EVANS, Materials Science Program and Department of Materials Science and Engineering, University of Wisconsin Madison, FRANZ J. HIMPSEL, Department of Physics, University of Wisconsin Madison — The orientation of pentacene films on SiO2 is studied for the thickness range from a monolayer to 150 nm by polarization-dependent NEXAFS spectroscopy (Near Edge X-ray Absorption Fine Structure). All films exhibit a strong polarization dependence of the n* orbitals, which indicates that the pentacene molecules are highly ordered. However, the degree of orientation varies with the rate at which pentacene molecules are deposited. This difference can be explained by a previously-proposed mixture of the bulk phase and a metastable thin film phase. Faster rates favor the thin film phase and slower rates the bulk phase. Our NEXAFS results extend previous structural studies down to the first layer at the oxide interface, which is critical for the performance of devices. Including a finite distribution of the molecular tilt angles in the data analysis accounts for residual disorder. Damage to the molecules by hot electrons from soft x-ray irradiation eliminates the splitting between nonequivalent n* orbitals, indicating a breakup of the pentacene molecule.
of about 2.0 eV, which is attributed to the edges of HOMO and LUMO bands of the molecules. Measurements over a wide range of tunnel currents are in

nm indicating that the Pn molecules are standing up, confirming the relatively weak interaction between the substrate and the film. STS reveals a band gap

electronically decouples the molecular films from the substrate. Scanning tunneling microscopy (STM) and spectroscopy (STS) was performed at room tem-

SiC surfaces etched at 1600˚C in 1 atm of hydrogen to form atomically flat substrates for Pn deposition. Oxidizing these substrates prior to Pn deposition

, SANDEEP GAAN, ROBERTO DUCA, RANDALL FEENSTRA, Carnegie Mellon University — Among various organic semiconductors,

to the modulation of the transfer integrals were found to display large nonlinear electron-phonon couplings. In the case of oligoacene crystals several phonon modes that contribute most strongly

phonon interaction will be discussed in detail. Our results show that for an adequate description of the charge transport in organic semiconductors both local

Institute of Technology — In this contribution we will discuss the present state-of-the-art in the derivation of electronic and electron-phonon coupling constants in

organic semiconductors from quantum-chemical calculations. We will reveal some of the shortcomings of the current models used to depict organic semiconductors and also the paths to be followed to achieve significant improvements. The contributions of both intra-molecular and inter-molecular vibrations to the electron-

phonon interaction will be discussed in detail. Our results show that for an adequate description of the charge transport in organic semiconductors both local and non-local electron-phonon mechanisms should be taken into account. In the case of oligoacene crystals several phonon modes that contribute most strongly to the modulation of the transfer integrals were found to display large nonlinear electron-phonon couplings.

1 The National Science Foundation supported this work under Award No. DMR-0348354. CHESS is supported by the National Science Foundation and the National Institutes of Health/National Institute of General Medical Sciences under Award No. DMR-0225180.

1:39PM B17.00011 Charge-Transport Parameters in Molecular Organic Semiconductors.

, YINA MO, Department of Physics, Harvard University, PAUL MARAGAKIS, Department of Chemistry, Harvard University, EFTHMIOS KAXIRAS, Department of Physics and Division of Engineering and Applied Sciences — We study the energetics and dynamics of pentacene molecules in vacuum and saturated diamond (111) surface and silica surfaces. Force field molecular dynamics simulations are applied to capture the van de Waals type interactions among the pentacene molecules and the substrates. The herringbone arrangement of the molecules is found to be optimal both in vacuum and on various inert surfaces. A 90 degree rotation of the entire structure relative to that experimentally reported is identified on the silica surfaces.

1:51PM B17.00012 Scanning Tunneling Microscopy and Spectroscopy of Pentacene films Deposited on SiC.

, SANDEEP GAAN, ROBERTO DUCA, RANDALL FEENSTRA, Carnegie Mellon University — Among various organic semiconductors, pentacene (Pn) has attracted much attention because of its ability of form ordered structures and its relatively high electron and hole mobilities. We have used SiC surfaces etched at 1600 °C in 1 atm of hydrogen to form atomically flat substrates for Pn deposition. Oxidizing these substrates prior to Pn depositionelectrocally decouples the molecular films from the substrate. Scanning tunneling microscopy (STM) and spectroscopy (STS) was performed at room tempera-
ture on in-situ deposited Pn films. STM reveals a dendritic morphology of the films, consistent with prior reports [1]. We find a step height of 1.43±0.10 nm indicating that the Pn molecules are standing up, confirming the relatively weak interaction between the substrate and the film. STS reveals a band gap of about 2.0 eV, which is attributed to the edges of HOMO and LUMO bands of the molecules. Measurements over a wide range of tunnel currents are in progress, in an effort to deduce any transport limitations in the films. Supported by NSF. [1] F.-J. Meyer zu Heringdorf et al., Nature 412, 517 (2001)

2:03PM B17.00013 Time Resolved Microscopy of Charge Trapping in Polycrystalline Pentacene.

, MICHAEL JAQUITH, Cornell University, ERIK MULLER1, Brookhaven Natl. Labs, JOHN MAROHN, Cornell University — The microscopic mechanisms by which charges trap in organic electronic materials are poorly understood. Muller and Marohn recently showed that electric force microscopy (EFM) can be used to image trapped charge in working pentacene thin-film transistors [E. M. Muller et al., Adv. Mater. 17 1410 (2005)]. We have made a new discovery by imaging trapped charge in pentacene films with much larger grains. In contrast to the previous study in which charge was found to trap inhomogeneously throughout the transistor gap, we find microscopic evidence for a new trapping mechanism in which charges trap predominantly at the pentacene/metal interface in large-grained devices. We conclude that at least two charge trapping mechanisms are at play in polycrystalline pentacene. We have made localized measurements of the trap growth over time by performing pulsed-gate EFM experiments. Trap formation is not instantaneous, taking up to a second to complete. Furthermore, the charge-trapping rate depends strongly on gate voltage (or hole concentration). This kinetics data is consistent with the hypothesis that traps form by chemical reaction.

1 Previously at Cornell University

Monday, March 5, 2007 11:15AM - 2:15PM

Session B20 DMP: Focus Session: Properties of Ferroelectrics and Relaxors

Colorado Convention Center 105
soft mode implies a strong interaction between the soft mode and the additional mode. In the first order spectrum is due to the zone folding in structures with strain, defect and disorder. This additional mode, like soft mode, also significantly

in the first order Raman spectrum of ferroelectric PbZr$_x$O$_3$. MATTHEW G. HILT, K.A. PESTKA II

films deposited on MgAl$_2$O$_3$ substrate a 1st order phase transition was observed and for KTN 1x1 super

11:51AM B20.00004 Interaction of Terahertz Radiation with Ferroelectrics, KEITH NELSON, Department of Chemistry, MIT — Ferroelectric crystals have long been used as acoustic transducers and receivers. An extensive toolset has been developed for MHz-frequency acoustic wave generation, control, guidance, and readout. In recent years, an analogous toolset has been developed for terahertz wave transduction and detection. Femtosecond optical pulses irradiate ferroelectric crystals to generate responses in the 0.1-5 THz frequency range that are admixtures of electromagnetic and polar lattice vibrational excitations called phonon-polaritons. Spatiotemporal femtosecond pulse shaping may be used to generate additional optical pulses that arrive at specified times and sample locations for control and manipulation of the THz waves. Femtosecond laser machining may be used for fabrication of waveguides, resonators, and other structures that are integrated into the ferroelectric host crystal. Finally, real-space imaging of the THz fields can be executed with variably delayed femtosecond probe pulses, permitting direct visualization of THz wave spatial and temporal evolution. This “polaritonics” toolset enables multiplexed generation of arbitrary THz waveforms and use of the waveforms within the ferroelectric host crystal or after projection into free space or an adjacent medium. The polaritonics platform will be reviewed and several new developments and applications will be presented. These include spectroscopy of terahertz ferroelectrics, whose temperature-dependent dielectric responses in the GHz-THz regime reveal complex polarization dynamics on well separated fast and slow time scales; direct measurement of phonon-polariton lattice vibrational displacements through femtosecond time-resolved x-ray diffraction; generation of high polariton field amplitudes and pulse energies; use of large-amplitude polariton waves to drive nonlinear lattice vibrational responses; and enhancement of optical-to-THz conversion efficiency through a pseudo-phase-matching approach that circumvents the very large disparity between refractive index values at optical and THz frequencies.

12:27PM B20.00005 Elastic constants and sound velocities in single crystal transition metal scandates, MATTHEW G. HILT, K.A. PESTKA II, JIN H. SO, J.D. MAYNARD, The Pennsylvania State University — An important effect on thin films deposited on substrates is the strain induced by lattice mismatch. Different perovskite structured transition metal scandates have similar a-axis lattice parameters but slightly different c-axis lattice parameters. By adjusting the transition metal content, the c-axis lattice parameter may be controlled, so that if these materials are used as substrates, lattice mismatch may be greatly reduced. To further match lattices dynamically, it is necessary to know the elastic constants of the scandate materials. However, only small single crystals of GdScO$_3$, DyScO$_3$, SmScO$_3$, and NdScO$_3$ have been fabricated. By using the small sample version of resonant ultrasound spectroscopy, we have determined the elastic constants and sound velocities for several transition metal scandates.

12:39PM B20.00006 Additional mode of PbZr$_x$Ti$_{1-x}$O$_3$ films, CHI YAT YAU, Department of Physics, Florida International University, Miami, Florida 33199. RELVA BUCHANAN, Department of Chemical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio 45221-0012 — In addition to the phonon modes predicted by the selection rule, a phonon mode at 45 cm$^{-1}$ (lower than soft mode frequency) was observed in the first order Raman spectrum of ferroelectric PbZr$_x$Ti$_{1-x}$O$_3$ films with $x = 0 - 1$. Thus, this additional mode is not a zone-center mode. Its existence in the first order spectrum is due to the zone folding in structures with strain, defect and disorder. This additional mode, like soft mode, also significantly downshifts as approaching the phase boundaries, e.g. at $x = 0.5$ and 0.95, or with the grain size change. The similar change of the additional mode and the soft mode implies a strong interaction between the soft mode and the additional mode.

1This work is supported by a NSF Grant: NSF-ECS-0100199.
12:51PM B20.00007 Phonon anomalies induced by polar nano-regions in a relaxor ferroelectric, GUANGYONG XU, Brookhaven National Laboratory, JINSHEng WEN, Brookhaven National Lab/Stonybrook University, CHRIS STOCK, Johns Hopkins University, PETER GEHRING, National Institute of Standards and Technology — Inelastic neutron scattering was used to measure both acoustic and optic phonons polarized along (110) (T2 mode) in the relaxor ferroelectric compound PZN-4.5PT. In the low temperature rhombohedral phase, a single domain state was achieved by cooling the single crystal sample under an external electric field of 2 kV/cm along the [111] direction. Phonon measurements were performed near the (2,2,0) and (2,0,2) Bragg peaks. We have found that the T2 phonon couples closely to the diffuse scattering, which arises from polar nano-regions in the system. With the redistribution of diffuse scattering under the external field (see Ref. 1), a clear hardening of T2 mode was observed near the (2,0,2) Bragg peak, while the T2 mode near (2,2,0) Bragg peak softens significantly and becomes over-damped. Our results indicate local inhomogeneities such as the PNR can have direct and significant effects on the lattice dynamics and stability of the whole system. Ref. 1: “Electric-field-induced redistribution of polar nano-regions in a relaxor ferroelectric”, Guangyong Xu, Z. Zhong, Y. Bing, Z.-G. Ye, and G. Shirane, Nature Materials 5, 134, (2006).

1:03PM B20.00008 Cubic ground state of field-cooled PbMg1/3Nb2/3O3 1, PETER GEHRING, National Institute of Standards and Technology, CHRIS STOCK, Johns Hopkins University, GUANGYONG XU, Brookhaven National Laboratory, HAOSU LUO, Chinese Academy of Sciences, HU CAO, JIEFANG LI, DWIGHT VIEHLAND, Virginia Tech, GEN SHIRANE 2, Brookhaven National Laboratory — Neutron and x-ray diffraction techniques have been used to study the competing long and short-range polar order in the relaxor PbMg1/3Nb2/3O3 (PMN) under the influence of an external [111]-oriented electric field. While the bulk unit cell remains cubic for electric fields up to 8 kV/cm, a suppression of the diffuse scattering and a concomitant enhancement of the Bragg peak intensity is observed below Tc = 210K, indicating a more ordered structure with increasing electric field yet an absence of a long-range ferroelectric ground state. The electric field strength has little effect on the diffuse scattering above Tc. The absence of hysteresis suggests that the ground state of PMN may not be a frozen glassy phase, but may be better understood in terms of random fields introduced through the presence of structural disorder.

1:15PM B20.00009 Dielectric Spectroscopy and conductivity relaxation of PSN-PST relaxor thin films, MARGARITA CORREA, NATASAN BASKARAN, RAM KATIYAR, Department of Physics, University of Puerto Rico, San Juan PR00931-3343 — abstract—Relaxor ferroelectric materials exhibit singular dielectric relaxation. They have large dielectric constant, high piezo and electrostrictive coefficients that make them useful for sensors, actuators and ferroelectric related devices. We have prepared PSN-PST relaxor thin films by pulsed laser deposition technique. Studies of dielectric properties, as a function of temperature (100-650K) and frequency (40 Hz –1 MHz) have shown that the materials have diffuse phase transition along with the frequency dispersion. The magnitude of dielectric constant and the temperature of maximum permittivity (Tm) differ from those in the bulk form. However, its conductivity behavior follows similar trend in both bulk and thin film forms. The ac conductivity exhibits frequency independent plateau at lower frequencies followed by a dispersion region at higher frequencies. The observed dispersion of conductivity with frequency can be described by a power law σ(ω) = σdc + Aω^n, with n>1. The unusual high n value is due to glassy like nature of the relaxor system and it is explained in terms of polaron assisted ionic mechanism. Detailed results will be presented.

1:27PM B20.00010 Quantitative Huang-scattering analysis of local structure in the relaxor-based piezoelectric PZN-4.5%PT 1, BRANTON J. CAMPBELL, VAYEE VUE, DANIEL ROBERTSON, Brigham Young University, Dept. of Physics & Astronomy, STEPHAN ROSENKRANZ, Argonne Nat. Lab., Mat. Sci. Div., PETER LEE, Argonne Nat. Lab., Advanced Photon Source, STINE N. ANACONA, RAY OSSBORN, Argonne Nat. Lab., Mat. Sci. Div. — Polar nano-regions (PNR) in ferroelectric relaxor materials like Pb(Zn1/3Nb2/3)O3 and Pb(Mg1/3Nb2/3)O3 are of pressing applied interest due to their influence on the remarkable piezoelectric properties of their solid solutions with PbTiO3. In the recent literature, x-ray and neutron single-crystal diffuse scattering techniques have been shown to provide qualitative insight into the local structure of these materials. Here, we present a quantitative three-dimensional Huang-scattering analysis of 80 keV x-ray single-crystal diffuse scattering data from PZN-4.5%PT.

1:39PM B20.00011 NMR Observation of Impurity-Pair Ordering in Weakly Disordered Solid Solutions 1, DAVID AILION, University of Utah, Department of Physics, BOSTJAN ZALAR, ANDRJJA LEBAR, J. Stefan Institute, Ljubljana, Slovenia — Breaking of the average cubic symmetry in Li-doped potassium tantalate (K1-xLi_xTaO3) was observed with quadrupole-perturbed 7LiNMR at temperatures (150-400 K) far above the nominal glass transition temperature (80 K). The observed spectrum consists of contributions from both isolated Li ions (i.e., with no nearest neighbor Li) and from Li pairs. The isolated Li ions move among six equivalent off-center sites in a potential having cubic symmetry. These have zero average electric-field gradient and, hence, exhibit no quadrupole splitting. In addition, very low intensity, but well resolved, quadrupole satellites having a temperature-dependent splitting were observed. This splitting indicates that the various Li pair configurations are not all equally probable. These are the first observations of biased Li-ion ordering that persists in the paraelectric phase at temperatures high above the glass phase.

1:51PM B20.00012 Local Basis Set Superelliptical Studies of (K,Na)NbO3 Solid Solutions, RICARDO KAGIMURA, MALLIGA SUEWATTANA, DAVID J. SINGH, Oak Ridge National Laboratory — We report density functional supercell calculations for (K,Na)NbO3 perovskite solid solutions using the local basis SIESTA code. We did detailed comparisons of results for ferroelectric structures and vibrational frequencies obtained with SIESTA with those obtained using all-electron full potential LAPW calculations, and used these comparisons to establish compact but accurate choices of basis set and pseudopotentials for the SIESTA calculations. Supercell calculations using SIESTA are used to investigate the dependence of ferroelectric polarization and local structure on the K/Na ordering. This work was supported by the DOE ORNL LDRD program and the Office of Naval Research.
2:03PM B20.00013 Effect of elastic strain and Sc dopant concentration-dependent cell volume on the electrical properties of Epitaxial (Ba,Sr)TiO$_3$ thin films, WOOYOUNG PARK, CHEOLSEONG HWANG, Seoul National University, Korea, JOHN D. BANIECKE, MASATOSHI ISHI, KAZUAKI KURIHARA, KAZUNORI YAMANAKA, Fujitsu Laboratories Ltd., Atsugi, Japan, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM, FUJITSU LABORATORIES LTD; TEAM — We present the results of a systematic study of the correlation between dopant concentration-dependent elastic strain and dielectric properties in (Ba,Sr)TiO$_3$ films. For this work, undoped and Sc-doped (Ba,Sr)TiO$_3$ thin film capacitors epitaxially grown on SrTiO$_3$ substrate were prepared by a sputter deposition method. Sc-doped BST capacitors exhibit significantly higher permittivity and lower leakage current density, but little effect on the loss tangent, as compared to nominally undoped BST capacitors. The Ti/(Ba+Sr) ratio of the films and Sc dopant concentration-dependent unit cell volume, as determined by x-ray sin$^{2}\psi$ analysis, are consistent with the preferential B-site occupancy of the Sc dopant. Furthermore, this work suggests that dopant concentration-dependent elastic strain as well as the 2D clamping effect of thin films on a thick substrate must be considered to fully understand the dielectric behavior of perovskite titanate thin films. 1. N. A. Pertsev, A. G. Zembligotov, and A. K. Tagantsev, Phys. Rev. Lett. 80, 1988 (1998)

Monday, March 5, 2007 11:15AM - 2:15PM
Session B23 DMP DCOMP: Focus Session: High Pressure II - Earth and Planetary Materials
Colorado Convention Center 110

11:15AM B23.00001 High-pressure investigations of Earth's interior, JENNIFER JACKSON, Caltech — In the first half of the talk, the electronic structure of iron in ferromagnesium silicate perovskite will be discussed. Knowledge of iron valences and spin states in silicate perovskite is relevant to our understanding of the physical and chemical properties of Earth's lower mantle such as transport properties, mechanical behavior, and element partitioning. In this study, we have measured the electronic structure of the iron component of an aluminous Fe-bearing silicate perovskite sample, (Mg$_{0.84}$Fe$_{0.16}$)$_2$SiO$_4$, close to a pyrolite composition, using synchrotron Mössbauer spectroscopy (SMS) and laser heated diamond anvil cells at high-pressure and temperatures at sample 3-ID of the Advanced Photon Source. Evaluation of the spectra provided the isomer shift and the quadrupole splitting of the iron component in silicate perovskite, which gives information on valence and spin states under lower mantle conditions. In the second half of the talk, experiments on the melting curve of iron at high-pressures will be presented. Seismological observations indicate that Earth's iron-dominated core consists of a solid inner region surrounded by a liquid outer core. Previously, melting studies of iron metal at high-pressures and temperatures were performed by shock-compression, resistive- and laser-heating in diamond anvil cells using visual observations or synchrotron x-ray diffraction and theoretical methods. However, the melting curve of iron is still controversial. Here, we will present a new method of detecting the solid-liquid phase boundary of iron at high-pressure using SMS. The characteristic SMS time signature is observed by fast detectors and vanishes suddenly when melting occurs. This process is described by the Lamb-Mössbauer factor $f = \exp(-k_2^2 - x^2)$, where $k$ is the wave number of the resonant x-rays and $x^2$ is the mean-square displacement of the iron atoms.

11:51AM B23.00002 Infrared Reflectance of Magnesiowustite(Mg$_{1-x$Fe}$_x$O): Experiment and Theory, TAO SUN, PHILIP B. ALLEN, Department of Physics and Astronomy, SUNY at Stony Brook, DAVID G. STAHNKE, Department of Physics, University of California, San Diego, STEVEN D. JACOBSEN, Department of Earth and Planetary Sciences, Northwestern University, CHRISTOPHER C. HOMES, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory — We measured the optical reflectance spectra(0°-3230 cm$^{-1}$) of magnesiowustite(Mg$_{1-x$Fe}$_x$O, $x$=0.06, x=0.27) at 6K and 295K, using a Bruker IFS 113v spectrometer. Kramers-Kronig relations are used to extract the corresponding dielectric functions. The Infrared parts of the spectra resemble those of pure MgO, while showing much smaller temperature dependence. There are two factors determining the structure of dielectric functions: a) anharmonic phonon-phonon interactions, b) disorder scattering. A breathing-shell model is used to evaluate factor a) in pure MgO, and a supercell is built to estimate the influence of factor b) in Fe doped MgO. Our results will be useful for computing the heat conductivity of magnesiowustite in the earth's lower mantle.

12:03PM B23.00003 Dynamical mean-field theory study of the high pressure behavior of FeO$^{1}$, A.C. KOLLIAS, R.E. COHEN, Carnegie Institution of Washington — First-principles calculations have an important part in the development of our understanding of Earth's interior, including geophysical and geochemical phenomena. Proper treatment of iron bearing minerals is fundamental in this respect. Unfortunately standard density functional theory (DFT) approaches such as the local density (LDA) or the generalized gradient approximations (GGA) fail in describing qualitative features of simple iron containing minerals; for example the insulating nature and magnetic structure of many metal oxides such as FeO. The LDA+U approximation, self-interaction correction (SIC), and dynamical mean-field theory (DMFT) have demonstrated significant improvement in the physical description of transition metal and rare earth compounds. Presented results will focus on theoretical predictions obtained with the DMFT method. The high pressure behavior and high-spin-low-spin phase transition for iron oxide in the distorted rocksalt (B1) structure.

3 Research Supported by the National Science Foundation

12:15PM B23.00004 Elastic Signature of the High-Spin to Low-Spin Transition in Magnesiowüstite$^{1}$, CESAR DA SILVA, RENATA WENTZCOVITCH, CEMS and MSI, University of Minnesota, Minneapolis, USA, TAKU TSUCHIYA, Geodynamics Research Center, Ehime University, Matsuyama, Japan — It has been reported that the high to low-spin spin transition in ferrous iron in magnesiowustite (Mw) under pressure is accompanied by considerable volume reduction and changes in elastic properties. Using an LDA+U method with consistently calculated (Mw) under pressure is accompanied by considerable volume reduction and changes in elastic properties. Using an LDA+U method with consistently calculated parameters, we investigated the elastic signature of the spin transition in Mg$_{1-x$Fe}$_x$O with parameters relevant to Earth's lower mantle. Equations of state are fit for a range of compositions and used to predict the Fe$^{2+}$ high- to low-spin transition pressure and associated changes in volume and bulk modulus. We predict a relatively constant transition pressure for $x < 0.25$, but a significant decrease for higher Fe concentrations, contrary to the trend for rocksalt (Fe$_2$O), suggesting the mechanism for spin transition is highly dependent on the structural environment of Fe. The spin transition is dominated by both the spin flip energy and the change in volume from high- to low-spin. Furthermore, volume trends show that high-spin Fe$^{2+}$ is larger than Mg$^{2+}$ even under pressure, but low-spin Fe$^{3+}$ is smaller at ambient conditions and approximately the same size as Mg$^{2+}$ under pressure, which has implications for correctly calculating Fe partitioning coefficients in the lower mantle. We also find the spin transition pressure differs between Fe$^{2+}$ and Fe$^{3+}$; therefore the coupling behavior of these two species must be examined closely.

3 Research supported by NSF/EAR 013533, NSF/EAR 0230319, and NSF/ITR 0428774

12:27PM B23.00005 ABSTRACT WITHDRAWN

12:39PM B23.00006 Ab initio Study of the Composition Dependence of the Pressure-Induced Spin Transition in Perovskite (Mg,Fe)SiO$_3$, AMELIA BENGTSON, University of Wisconsin - Madison, KRISTIN PERSSON, MIT, DANE MORGAN, University of Wisconsin - Madison — We present ab initio calculations of the zero-temperature compositional dependent spin transition in (Mg,Fe)SiO$_3$ perovskite at pressures relevant to Earth's lower mantle. Equations of state are fit for a range of compositions and used to predict the Fe$^{2+}$ high- to low-spin transition pressure and associated changes in volume and bulk modulus. We predict a relatively constant transition pressure for $x < 0.25$, but a significant decrease for higher Fe concentrations, contrary to the trend for rocksalt (Fe$_2$O), suggesting the mechanism for spin transition is highly dependent on the structural environment of Fe. The spin transition is dominated by both the spin flip energy and the change in volume from high- to low-spin. Furthermore, volume trends show that high-spin Fe$^{2+}$ is larger than Mg$^{2+}$ even under pressure, but low-spin Fe$^{3+}$ is smaller at ambient conditions and approximately the same size as Mg$^{2+}$ under pressure, which has implications for correctly calculating Fe partitioning coefficients in the lower mantle. We also find the spin transition pressure differs between Fe$^{2+}$ and Fe$^{3+}$; therefore the coupling behavior of these two species must be examined closely.
12:51PM B23.00007 First-principles investigation of the spin state of ferrous iron in MgSiO$_3$ under pressure$^1$, **YONGGANG YU**, CEMS, University of Minnesota, **RYAN REQUIST**, Friedrich Alexander University Erlangen 91058, Germany, **KOICHIRO UMEMOTO**, RENATA WENTZCOVITCH, MSI and CEMS, University of Minnesota — We present a density functional study of the pressure induced spin transition in ferrous iron in MgSiO$_3$ perovskite and post-perovskite. We address the influence of iron concentration and configuration (structural and magnetic), as well as technical issues such as the nature of the exchange correlation (XC) functional (LDA versus PBE-GGA) on the spin transition pressure. Supercells containing up to 160 atoms were adopted to tackle these issues. We show that there are preferred configurations for high-spin and low-spin iron and that the spin transition pressure depends strongly on iron concentration and XC functionals. We also address the possibility of a structural change accompanying the spin transition.$^1$

$^1$Research supported by NSF/EAR 013533, 0230319, and NSF/ITR 0428774 (VLab). Computations were performed at the Minnesota Supercomputing Institute and Indiana University's BigRed system.

1:03PM B23.00008 Structure and freezing of MgSiO$_3$ liquid in Earth’s interior, **LARS STIXRUDE**, University of Michigan, **BIJAYA KARKI**, Louisiana State University — Silicate liquids are primary agents of mass and heat transport, yet little is known of their physical properties or structure over most of the mantle pressure regime. We have applied density functional theory within the local density approximation to the study of silicate liquids via Born-Oppenheimer first principles molecular dynamics. The simulations are performed in the NVT ensemble with a Nose thermostat. We find that over the pressure regime of Earth’s mantle the mean Si-O coordination number increases nearly linearly with compression from four-fold to six-fold. The Grüneisen parameter of the liquid increases markedly on compression, in contrast to the behavior of mantle crystalline phases, and in accord with expectations based on the pressure-induced change in structure of the liquid. The density contrast between liquid and crystal decreases nearly five-fold over the mantle pressure regime and is 4 % at the core-mantle boundary. The melting curve, obtained via integration of the Clausius-Clapeyron equation yields a melting temperature of 5400 ± 600 K at the core mantle boundary. Our results support the notion of buoyantly stable silicate melts at the core-mantle boundary.

1:15PM B23.00009 Consequences of the Quasiharmonic Approximation: Tests and Predictions$^1$, **PIERRE CARRIER**, Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science, University of Minnesota, **JUN TSUCHIYA**, Geodynamics Research Center, Ehime University, Matsuyama, Japan, **RENATA M. WENTZCOVITCH**, Minnesota Supercomputing Institute, Department of Chemical Engineering and Materials Science, University of Minnesota — The quasiharmonic approximation (QHA) is extremely useful since it allows the computation of thermodynamic properties if one knows the volume dependence of the vibrational density of states. It has an important consequence: the structure and vibrational properties of the solid depend on volume alone. The temperature dependence occurs via extrinsic volumetric effects. We present here a criterion to determine the pressure- temperature range of validity of the QHA, apply it to and test it in MgSiO$_3$-perovskite, and inspect the possibility of a simple volumetric depended of other properties such as acoustic velocities, i.e., “Birch’s Law.”$^1$

$^1$Research supported by NSF/EAR and NSF/ITR programs

1:27PM B23.00010 Quantum Monte Carlo Benchmarks Functional for Silica Polymorphs, **K.P. DRIVER**, J.W. WILKINS, Ohio State U., **R.G. HENING**, C.J. UMRIGAR, Cornell U., **G. SCUSERIA**, Rice U., **B. MILITZER**, R.E. COHEN, Carnegie Institution of Washington — For many silica polytypes, the local density approximation (LDA) does a better job than the generalized gradient approximation (GGA) in predicting structural properties and bulk moduli. However, gradient corrections to the charge density are necessary for accurate phase energy differences. Functional go beyond GGA may improve the accuracy of both structures and energies. For example, a meta-GGA functional, TPSS, and hybrid functionals B3LYP and HSE have shown improvement in other systems. We compare results from these functionals for structural properties, energy differences, and bulk moduli for a few high pressure phases of silica, and benchmark the results with Quantum Monte Carlo. Preliminary QMC results indicate that careful wavefunction optimization and finite size effects are of particular importance in obtaining accurate silica phase properties. Supported by DOE(DFG02-99ER45795), NSF (EAR-0530301, DMR-0205328), and Sandia National Laboratory. Computation at OSC and NERSC.

1:39PM B23.00011 Quantum Monte Carlo Simulations of the Quartz to Stishovite Transition in SiO$_2$, **R.E. COHEN**, Carnegie Institution of Washington, **M.I. TOWLER**, PABLO LOPEZ RIOS, NEIL DRUMMOND, RICHARD NEEDS, TCM, Cavendish Laboratory, University of Cambridge, U.K. — The quartz-stishovite transition has been a long standing problem for density functional theory (DFT). Although conventional DFT computations within the local density approximation (LDA) give reasonably good properties of silica phases individually, they do not give the energy difference between quartz and stishovite accurately. The LDA gives stishovite as a lower energy structure than quartz at zero pressure, which is incorrect. The generalized gradient approximation (GGA) has been shown to give the correct energy difference between quartz and stishovite (about 0.5 eV/formula unit) (Hamann, PRL 76, 660, 1996; Zupan et al., PRB 58, 11266, 1998), and it was generally thought that the GGA was simply a better approximation than the LDA. However, closer inspection shows that other properties are not better for the GGA than the LDA, so there is room for improvement. A new density functional that is an improvement for most materials unfortunately does not improve the quartz-stishovite transition (Wu and Cohen, PRB 73, 235116, 2006). We are performing QMC computations using the CASINO code to obtain the accurate energy difference between quartz and stishovite to obtain more accurate high pressure properties, and to better understand the errors on DFT and how DFT can be improved.

$^1$Supported by NSF.

1:51PM B23.00012 First-principles calculations of thermodynamic properties and phase transitions in Al$_2$O$_3$ and Ga$_2$O$_3$ at high temperature and high pressure, **BIN XU**, **JIANJUN DONG**, Auburn University — Using ab initio density functional theory and statistical quasi-harmonic approximation theory, we have calculated thermodynamic potentials of mineral Al$_2$O$_3$ materials and the related Ga$_2$O$_3$ materials over a wide range of temperature and pressure (T-P) conditions. The equilibrium T-P phase diagrams are predicted to understand the trend of pressure induced phase transitions in group IIIB oxides. Furthermore, we theoretically explored the possible new high-pressure structures of Ga$_2$O$_3$. Finally, we derived experimentally measurable thermal properties, such as lattice thermal expansion, heat capacity, and isothermal compressibility. Our calculated thermal properties are in excellent agreement with available experiments.
2:03PM B23.00013 Proton behaviour, structure and elasticity of serpentine at high-pressure, MAINAK MOOKHERJEE, Yale University, LARS STIXRUDE, University of Michigan — Serpentine occurs in oceanic crust as the alteration product of ultramafic rocks and is a possible candidate for carrying water to the deep Earth. The presence of sub-surface serpentine may be manifested by mud volcanoes, high electrical conductivities, and seismic anomalies. Using density functional theory, we predict a phase transition in serpentine near 22 GPa. The phase transition is caused by a re-orientation of the hydroxyl vector coupled with changes in the di-trigonal rings of SiO$_4$ tetrahedra. The symmetry of the crystal-structure remains unaffected. Evidence of pressure-induced hydrogen bonding is absent in serpentine, as evident from the reduction of O-H bond length upon compression. Results of compression for the low-pressure phase is well represented by a fourth order Birch-Murnaghan finite strain expression with $K'_O = 63$ GPa, $K''_O = 10.2$ and $K''_O K''_O = -120$, where $K$ is the bulk modulus, prime indicates pressure derivatives, and O refers to zero pressure. At low pressures, the elastic constant tensor is highly anisotropic with $C_{11} = 2.4 \times C_{33}^0$, and becomes more isotropic with compression. We find an elastic instability near 36 GPa that may be related to experimentally observed amorphization.

Monday, March 5, 2007 11:15AM - 1:39PM —
Session B27 DMP DCOMP: Focus Session: Computational Nanoscience II-Methods and Applications —

11:15AM B27.00001 Kinetic Monte Carlo simulations of Ag(111) island coarsening$^1$, GIREDIS NANDIPATI, YUNSIC SHIM, JACQUES AMAR, University of Toledo, ALTAF KARIM, University of Delaware, ABDELKADER KARA, TALAT RAHMAN, University of Central Florida — The results of parallel kinetic Monte Carlo simulations of submonolayer island coarsening on the Ag(111) surface are presented. Our simulations are carried out using a large database of activation barriers which has been generated from previous self-learning kinetic Monte Carlo simulations of small and medium-size clusters. In this database, which includes both single-atom and multi-atom concerted moves, interactions between a central atom and all other adatoms within the first two nearest-neighbor rings are taken into account, while the symmetry of the (111) surface is also used. In order to reach extended time and length-scales we have implemented a novel parallel kinetic Monte Carlo scheme in which processor domains are dynamically assigned in order to minimize boundary events. Preliminary results using an open database corresponding to a true self-learning kinetic Monte Carlo simulation will also be presented.

$^1$Supported by NSF through grant CCF-042882622

11:27AM B27.00002 Self-Learning Off-Lattice Kinetic Monte Carlo method as applied to growth on metal surfaces$^1$, OLEG TRUSHIN, Institute of Microelectronics and Informatics RAS, Yaroslavl, Russia, ABDELKADER KARA, TALAT RAHMAN, University of Central Florida — We propose a new development in the Self-Learning Kinetic Monte Carlo (SLKMC) method with the goal of improving the accuracy with which the atomic mechanisms controlling diffusive processes on metal surfaces may be identified. This is important for diffusion of small clusters (2 - 20 atoms) in which atoms may occupy Off-Lattice positions. Such a procedure is also necessary for consideration of heteroepitaxial growth. The new technique combines an earlier version of SLKMC$^1$ with the inclusion of off-lattice occupancy. This allows us to include arbitrary positions of adatoms in the modeling and makes the simulations more realistic and reliable. We have tested this new approach for the case of the diffusion of small 2D Cu clusters on Cu(111) and found good performance and satisfactory agreement with results obtained from previous version of SLKMC. The new method also helped reveal a novel atomic mechanism contributing to cluster migration. We have also applied this method to study the diffusion of Cu clusters on Ag(111), and find that Cu atoms generally prefer to occupy off-lattice sites. [1] O. Trushin, A. Kara, A. Karim, T.S. Rahman Phys. Rev B 2005

$^1$work supported by NSF-ITR 0428826

11:39AM B27.00003 Diffusion Limited Processes Using Accelerated Molecular Dynamics$^1$, ERDIAL BLEDIA, XING GAO, MURRAY DAW, Department of Physics and Astronomy / Clemson University — We present a systematic microscopic approach to diffusion-limited processes for intermetallic alloys using Accelerated Molecular Dynamics. On-the-fly kinetic Monte Carlo is combined with the Dimer Method to find the saddlepoints exiting a valley, based on energetics from the Embedded Atom Method. With this technique, we compute the tracer diffusivities as a function of composition and temperature for strongly ordered (Cu$_2$Au), weakly ordered (Ag-Au) and weakly clustered (Cu-Ni) alloys.

$^1$NSF-ITR

11:51AM B27.00004 Extension of Mean-Field Nuclearation Theory with Long-Range Interactions, JOHN A. VENABLES, JAMES DEGRAFFENREID, Dept. of Physics, Arizona State University, RAMON GRIMA, Institute for Mathematical Sciences, Imperial College, London, UK — Mean-field nuclearation theory is an important tool in understanding various adsorbate-substrate systems, particularly in the context of epitaxial growth. Conventional mean-field theory does not take into account nonlocal interactions, but these can be important in the nucleation and growth of various nanostructures. An approach due to Ovesson [1] is based on the assumption that the change of saddle-point energy in a potential field equals the average changes at the neighboring binding sites, but this assumption is not generally satisfied. We reformulate the theory in a more general sense, as an extension of the work of Grima and Newman [2] and Venables et al. [3]. This leads to a continuum mean-field description in a general potential field, in which the transport coefficients are intrinsically connected with the interaction potential and with microscopic parameters. Computational examples are presented for Ge/Si(001) material parameters.

[1] S. Ovesson, PRL 88, 116102 (2002);
12:03PM B27.00005 Capture-Zone Areas & the Wigner Distribution: New Case of Universal Scaling of Spacings in Fluctuating Systems, A. PIMPINELLI, UBP-Clermont 2 (France) & UM, T.L. EINSTEIN, U. of Maryland — When investigating scaling of island sizes during growth in d dimensions, one should consider the distribution of the areas of proximity cells around nucleation centers, i.e. capture zones (CZ). Using data from kinematic Monte Carlo studies we find that the CZ distributions in both d = 1 and d = 2 are well described by the generalized Wigner distribution (GWD) from random-matrix theory: $P_d(x) \propto a^d e^{-b/2}$. $P_d(x)$ accounts for a broad range of fluctuation phenomena, including the terrace-width distribution (TWd) on vicinal surfaces. For CZ distributions, we find $g = d/2$, where $i$ is the critical nucleus size. We present a phenomenological justification by constructing a Langevin equation similar to that used in accounting for the equilibration of TWds. We discuss implications for processing and analysis of experimental data.

1 Supported by NSF MRI SEC Grant DMR 05-20471, partially by DOE CMSN grant DEFG0205ER46227 (TLE) and CNRS Travel Grant (AP)

2 Mulheran et al., PRB 53 (96) 10261, 54 (96) 11681; EPL 49 (96) 617, 65 (04) 379. Amar, Family, et al., PRL 74 (95) 2006; PRB 64 (01) 205404. Evans, Bartelt, et al. PRB 66 (02) 235410; SSR 61 (99) 1.

3 A. Pimpinelli, H. Gebremariam, & T.L. Einstein, PRL 95 (95) 246101

12:15PM B27.00006 Feature detection for large-scale molecular dynamics simulations, HYOUNGKI PARK, Ohio State University, DAVID RICHELIE Stone Ridge Technology, JEONGMIM KIM, University of Illinois at Urbana-Champaign, JOSEPH GORSE, Battelle Memorial Inst, JOHN WILKINS, Ohio State University — Advances in computer hardware and numerical methods compound the analysis of complex, large-scale evolutionary phenomena. Progress comes from just-in-time analysis and data compression. Real-time multiscale analysis solution (RTMRA) on dynamical quantities (e.g., positions and local energies of atoms) based on Haar wavelets compress data more than 100-fold while retaining 0.1 Å.m.s. resolution. Further, RTMRA techniques enable a sophisticated event detection scheme capable of identifying meta-stable structures and detecting infrequent events, e.g., structural transitions, in the presence of thermal noise. As an example, the dynamics over a broad temperature range of silicon defect systems yields visually clear diffusion mechanisms for small silicon interstitial clusters (single-, di-, and tri-interstitial), and in general, we identify the origin of 311 defects.

12:27PM B27.00007 Objective Molecular Dynamics, TRAIAN DUMITRICA, Department of Mechanical Engineering, University of Minnesota, RICHARD JAMES, Department of Aerospace Engineering, University of Minnesota — We present a generalization of periodic molecular dynamics that we term objective molecular dynamics. It is a method of doing molecular dynamics for a restricted set of atoms, nonperiodically mapping the time-dependent displacements of this small set of atoms onto the full, typically infinite structure, such that the full structure satisfies exactly the full, unconstrained set of equations of molecular dynamics subject to certain group-invariant initial conditions. The method is applicable to a wide variety of interesting molecular structures including the tails, capsids and other parts of many viruses, carbon nanotubes, many of the common proteins, C60 and many other nanostructures now being synthesized, especially via the process of self-assembly. Overall, the strength of the proposed symmetry-based approach is that (i) it reduces the computational effort per atom to zero; (ii) it is compatible with full quantum mechanics, and (iii) the implementation can be done in a general framework, allowing for simulations of a large class of structures. In addition, the scheme is ideal for obtaining nanomechanical responses since it allows for applying various mechanical deformations. The method is illustrated by simulations of carbon nanotubes.

12:39PM B27.00008 Decorrelation of samples in Quantum Monte Carlo calculations and applications to metallic nanoclusters, DANIEL NISSENBAUM, BERNARDO BARBIELLINI, ARUN BANSIL, Northeastern University — We discuss decorrelation of samples in Quantum Monte Carlo (QMC) ground-state energy calculations for large lithium and water nanoclusters and show how accurate results can be obtained without the need for decorrelating samples. The scaling of the integrated autocorrelation time is analyzed as a function of nanocluster size. $\tau$ is scaled to quadratically in Li nanoclusters, which adds a quadratic factor to the scaling of the total computation time in this metallic case, a factor which does not appear in computations of non-metallic H2O nanoclusters. We choose nanoclusters which are relatively large in the context of QMC to demonstrate the application of these techniques — lithium nanoclusters with up to 64 atoms and water nanoclusters with up to 20 molecules.

1 Work supported in part by the USDOE.

12:51PM B27.00009 Linear Scaling NanoScience Simulations for Petascale Computing, ZHENGJI ZHAO, LIN-WANG WANG, JUAN MEZA, LBNL — There are many large-scale nanoscience problems that require ab initio accurate total energy calculations and atomic relaxations. Unfortunately, the traditional direct ab initio method scales as $O(N^3)$, where $N$ is the number of atoms in the system, and most of the $O(N)$ methods studied in the last decade have various numerical convergence problems and computer parallelization issues. In this talk, we present an alternative $O(N)$ method which divides the whole system into small fragments. By combining the fragments in an ingenious pattern, the artificial boundary effects of the spatial division can be canceled out. As a result, the difference between this method and the direct ab initio calculation is smaller than errors introduced by other numerical approximations, and the method scales almost linearly to the number of processors. We have used this method to calculate nanostructures with more than ten thousand atoms using thousands of processors under the conventional plane-wave pseudopotential approach. We will demonstrate that this approach provides a practical way for future petascale computation in materials/nanomaterials science.

1 This work was supported by DOE under Contract No. DEAC02-05CH11231. It used the resources of NERSC.

1:03PM B27.00010 Including spin-orbit coupling in materials-specific studies of spin transport, A.A. STARIKOV, P.J. KELLY, University of Twente — Spin-orbit coupling (SOC) plays a crucial role in magnetoelectronics: it is the origin of anisotropic magneto-resistance (AMR), prevents half-metallic ferromagnets from having 100% spin polarization, gives rise to spin-flip scattering which ultimately destroys the spin polarization of a current in non-magnetic materials - to mention but a few of its effects. Nevertheless, it has been virtually ignored in theoretical transport studies. To redress this neglect, we have developed a method based upon Linearized Muffin-Tin-Orbitals suitable for studying spin-dependent transport in nanostructures which includes SOC and provides a framework for modeling layered magnetic systems with non-collinear magnetizations. As a first application and test of the method, we study the AMR effect in ferromagnetic alloys.

1:15PM B27.00011 Modeling the deformation of materials with stochastic fractal microstructure, M.A. SOARE, R.C. PICU, Rensselaer Polytechnic Institute — Many materials with heterogeneous multiscale fractal structure are found in nature. Examples include biological tissues and bone, some rock such as sandstones, and aero-gels. In such materials the amount of geometrical detail observed in the microstructure increases from scale to scale in a self-similar manner, they lack characteristic length scales and the Hausdorff dimension is smaller than that of the embedding space. Furthermore, the microstructure is multiscale and stochastic, in the sense that the generating operators that map the geometry from one scale to the next are stochastic. In this work, we develop a method by which boundary value problems can be solved for these complex multiscale materials with minimal computational effort. Use is made of the scaling properties of the geometry and of stochastic finite elements in which the solution is approximated using chaos polynomials. The talk will review the formulation and a number of examples used for verification.
the photoresponse show the presence of significant potential fluctuations on the micron length scale along these devices. A correlation between the spatial positions of weak D lines, when observed, and changes in the photoresponse. Comparisons of the Raman spectra and the intensity can be comparable to or stronger than that arising from the charge separation at the Schottky barriers. The Raman spectra show high quality CNTs with some from fluctuations all along the device. The magnitude of the photoresponse from defects such as tube crossings and fluctuations in the tube environment can be discussed.


Excited states and electro-optics of carbon nanotubes, PHAEDON AVOURIS, IBM T.J. Watson Research Center — We will discuss experimental and theoretical results on nanotube excited state production and luminescence through photoexcitation, electron-hole recombination and hot carrier impact excitation. The effects of an external electric field, as well as environmental effects on the absorption and emission spectra will be examined. Finally, nanotube photoconductivity and photovoltage and the role of the substrate and defects on these processes will be analyzed.

Benoit St-Antoine, Elyse Adam, Carla Aguirre, David Menard, Departement de genie physique, Ecole Polytechnique de Montreal, Richard Martel, Departement de chimie, Universite de Montreal — Carbon nanotubes network transistors (CNNT) open a promising route for the integration of nanotubes in electronics for that they circumvent major issues related to their fabrication. They also reduce device-to-device discrepancies because they combine the properties of an ensemble of nanotube species. Here, we investigated the optoelectronic properties of the CNNT fabricated from different nanotube diameter distribution. (1) E.S. Snow, P.M. Campbell, M.G. Ancona, Appl. Phys. Lett., 2005, 86, 033105.

Electrically driven thermal light emission from individual single-walled carbon nanotubes, Y.K. KATO, PRESTO, Japan Science and Technology Agency, D. MANN, A. KINKHABWALA, E. POP, J. CAO, X. WANG, L. ZHANG, Q. WANG, H. DAI, Department of Chemistry and Laboratory for Advanced Materials, Stanford University, J. GUO, Department of Electrical and Computer Engineering, University of Florida — Light emission from carbon nanotubes offer unique opportunities in nano-optoelectronics, because of their chirality dependent electronic structure, availability of high quality electrical contact, and very high aspect ratio. We study electrically- driven light emission from individual single-walled carbon nanotubes, including both quasi-metallic and semiconducting species. Our field effect transistor structure utilizes a clean, as-grown nanotube suspended across a trench, allowing for low contact resistance and good isolation from the substrate. The spectra from quasi-metallic nanotubes reveal pronounced peaks in the visible and infrared corresponding to E_{11} and E_{22} transitions. The emission rates show strong correlation with electrical power dissipated in the devices, consistent with thermally excited emission due to resistive heating. We observe similar behavior for the semiconducting devices, although elctroluminescence in these nanotubes has been explained by either carrier injection or impact excitation.

D. Mann et al., submitted for publication (2006).

Excited states and electro-optics of carbon nanotubes, PHAEDON AVOURIS, IBM T.J. Watson Research Center — We will discuss experimental and theoretical results on nanotube excited state production and luminescence through photoexcitation, electron-hole recombination and hot carrier impact excitation. The effects of an external electric field, as well as environmental effects on the absorption and emission spectra will be examined. Finally, nanotube photoconductivity and photovoltage and the role of the substrate and defects on these processes will be analyzed.

Benoit St-Antoine, Elyse Adam, Carla Aguirre, David Menard, Departement de genie physique, Ecole Polytechnique de Montreal, Richard Martel, Departement de chimie, Universite de Montreal — Carbon nanotubes network transistors (CNNT) open a promising route for the integration of nanotubes in electronics for that they circumvent major issues related to their fabrication. They also reduce device-to-device discrepancies because they combine the properties of an ensemble of nanotube species. Here, we investigated the optoelectronic properties of the CNNT fabricated from different nanotube sources and found bright electroluminescent (EL) emission. The EL is specific to the nanotube source and can be linked using absorption spectra to their diameter distribution. (1) E.S. Snow, P.M. Campbell, M.G. Ancona, Appl. Phys. Lett., 2005, 86, 033105.

Carbon nanotubes network transistors (CNNT) open a promising route for the integration of nanotubes in electronics for that they circumvent major issues related to their fabrication. They also reduce device-to-device discrepancies because they combine the properties of an ensemble of nanotube species. Here, we investigated the optoelectronic properties of the CNNT fabricated from different nanotube sources and found bright electroluminescent (EL) emission. The EL is specific to the nanotube source and can be linked using absorption spectra to their diameter distribution. (1) E.S. Snow, P.M. Campbell, M.G. Ancona, Appl. Phys. Lett., 2005, 86, 033105.

Localised Raman Spectra and Field Effect Properties of Long Carbon Nanotube Field Emission Transistors, JAMES TSANG, MARCUS FREITAG, PHAEDON AVOURIS, IBM T. J. Watson Research Center — The spatially resolved photoresponse, and Raman spectra of CVD grown carbon nanotube field effect transistors with channel lengths between 2 and 50 μm have been measured using conventional imaging techniques at photon energies between 1.4 and 2.7eV. A strong localized photoresponse including both the short circuit photocurrent and the high electrical power dissipated in the devices, consistent with thermally excited emission due to resistive heating. We observe similar behavior for the semiconducting devices, although elctroluminescence in these nanotubes has been explained by either carrier injection or impact excitation.

D. Mann et al., submitted for publication (2006).

Localised Raman Spectra and Field Effect Properties of Long Carbon Nanotube Field Emission Transistors, JAMES TSANG, MARCUS FREITAG, PHAEDON AVOURIS, IBM T. J. Watson Research Center — The spatially resolved photoresponse, and Raman spectra of CVD grown carbon nanotube field effect transistors with channel lengths between 2 and 50 μm have been measured using conventional imaging techniques at photon energies between 1.4 and 2.7eV. A strong localized photoresponse including both the short circuit photocurrent and the high electrical power dissipated in the devices, consistent with thermally excited emission due to resistive heating. We observe similar behavior for the semiconducting devices, although elctroluminescence in these nanotubes has been explained by either carrier injection or impact excitation.

D. Mann et al., submitted for publication (2006).
1:03PM B28.00006 Impact Excitation by Hot Carriers in Carbon Nanotubes, VASILI PEREBEINOS, PHAEDON AVOURIS, IBM - Watson — We find in Ref. 1 and 2, that the impact excitation processes in nanoscale devices are much more efficient than in conventional bulk semiconductors due to the enhanced Coulomb interaction in low dimensions. In semiconducting carbon nanotubes, we calculate the impact excitation rates to be 4-5 orders of magnitude larger than in bulk semiconductors [2]. The impact excitation rate is much higher in nanotubes than the impact ionization, which neglects electron-hole interaction of the produced electron-hole pair, while their difference is negligible in bulk materials. The angular momentum conservation law plays a crucial role in determining the threshold energy of the impact excitation. The spectra of the produced excitons depends strongly on the bias and not constrained by the dipole selection rule as in the photoluminescence. The triplet excitons have approximately equal probability to be produced, unlike 1/4 statistical fraction for the independently injected electrons and holes. [1] J. Chen, V. Perebeinos, M. Freitag, J. Tsang, Q. Fu, J. Liu, Ph. Avoiris, Science 310, 1171, 2005. [2] V. Perebeinos and Ph. Avoiris, Phys. Rev. B 74, 121410(R), 2006.

1:15PM B28.00007 Exciton Annihilation Processes in Individual Single-Wall Nanotubes1, ADITYA MOHITE, PRASANTH GOPINATH, HEMANT SHAH, BHASKAR NAGABHIRAVA, TANESH BANSAL, BRUCE ALPHENAAAR, University of Louisville — Field enhanced photocurrent measurements of individual single-wall nanotubes show that bound exciton dissociation occurs through two distinct processes. At low fields, the barrier to field ionization is not surmounted but bound carriers can still discharge by tunneling into the free carrier states. At high fields (approximately by the binding energy divided by the Bohr radius, or $E_b/r$) the bound excitonic state is destroyed. We measure the photocurrent of a SWNT capacitor, in which the nanotubes lie on a 100 nm oxide dielectric on doped silicon substrate. This allows us to apply extremely large electric fields across the nanotube. Excitons do not contribute to the photocurrent unless dissipation into free carrier states occurs. At fields below $1 \times 10^8 \text{ V/m}$ the exciton peak increases according to Fowler-Nordheim field dependence. At a field of approximately $1.2 \times 10^8 \text{ V/m}$ the photocurrent rapidly increases by more than an order of magnitude suggesting a huge increase in the exciton dissociation rate. This corresponds to the predicted field required for exciton annihilation to occur.

1Office of Naval Research Grant # GB000468.

1:27PM B28.00008 The role of intrinsic regions in nanotube photodiodes, DEREK STEWART, Cornell Nanoscale Facility — In this work, we consider the impact of intrinsic regions on transport in carbon nanotube diodes. Recently nanotube diodes have been fabricated in a split-gate geometry where a central intrinsic region separates two regions gated p-type and n-type, respectively. These devices show near ideal diode behavior and can also act as photodetectors. We use a self-consistent non-equilibrium Green’s function approach to examine how the central intrinsic layer width affects the properties of a nanotube p-i-n photodiode. The charge and potential along the diode are determined self-consistently for systems with different intrinsic layer widths. We find that the intrinsic region has little effect on the dark current in the device. However, as the size of the intrinsic region increases, the photocurrent grows as well. The presence of a central intrinsic region also leads to greater power conversion efficiency in nanotube photodiodes. These changes in the photocurrent can be related to charge redistribution caused by the introduction of the intrinsic layer. This leads to a reduction of the flat band regions near the leads, while unmasking the van Hove singularities in the central intrinsic region that enhance the photocurrent for higher photon energies. This effect is quite general and may be observed in similar p-n junctions (i.e. nanowires) where the density of states is quasi-one dimensional.

1:39PM B28.00009 Dependence of Raman-active modes on the external voltage in single-wall carbon nanotube thin films, GIOVANNI FANCHINI, GOKI EDA, HUSNU EMRAH UNALAN, MANISH CHHOWALLA, Materials Science and Engineering - Rutgers University — We report on Raman measurements under the application of an external voltage in gap-cell devices made by transparent and conducting single-wall carbon nanotube (SWNT) thin films [1]. Two different Raman excitation wavelengths (785 and 633 nm) were used. Application of voltage results in downshifts of the D and G modes and in reduction of their intensity. The intensities of the radial breathing modes increase with voltage in metallic SWNTs, while decreasing in semiconducting SWNTs. A model explaining the phenomenon in terms of both direct and indirect (Joule heating) effects of the field is proposed. Our work rules out the elimination of large amounts of metallic SWNTs in thin film transistors using high field pulses. Our results support the existence of Kohn anomalies in the Raman-active optical branches of metallic graphitic materials. Additional Raman measurements in SWNT thin film transistors at varying source-drain voltage and gate voltage will be presented as well. [1] G Fanchini, et al, submitted [2] S.Piscanec et al, PRL 93 (2004) 185503

1:51PM B28.00010 Absolute Absorptivity of Single-walled Carbon Nanotubes Employing a Pyroelectric Detector, KATHERINE HURST, National Institute of Standards and Technology, ANNE DILLON, National Renewable Energy Laboratory, JOHN LEHMAN, National Institute of Standards and Technology — Optical properties are important for determining fundamental characteristics of carbon single-walled nanotube (SWNT) samples including purity, chirality, and tube diameter. Previously, we have estimated the volume fraction of metallic versus semiconducting tubes for highly purified SWNT bucky-paper on a pyroelectric detector from spectral responsivity measurements and an effective medium approximation to determine the dielectric function (1). Pyroelectric detector-based measurements are based on the thermalization of photons within the SWNT coating and provide a robust technique for measuring absolute absorptivity at normal incidence. Alternatively, we perform transmissivity measurements of SWNTs by employing a gold-black coated pyroelectric detector. Spectral responsivity measurements are made by direct substitution against a NIST calibrated detector such that quantitative changes in the volume fraction and purity of SWNT samples are revealed. These results will be compared to specular transmission measurements made by UV-VIS spectrometry. Raman spectroscopy will also serve to verify nanotube properties. (1) K.E.H. Gilbert, J.H. Lehman, A.C. Dillon and J.L. Blackburn Appl. Phys. Lett. 88, 143122 (2006).

2:03PM B28.00011 Photoresponse of Suspended Carbon Nanotube Networks: Single-Walled Carbon Nanotube Infrared Bolometer1, MIKHAIL E. ITKIS, FERENC BORONDICS, AIPING YU, ROBERT C. HADDON, Center for Nanoscale Science and Engineering, University of California, Riverside, CA 92521-0403 — The photoresponse of a single-walled carbon nanotube (SWNT) film is dramatically enhanced when the nanotube film is suspended between electrical contacts in vacuum. We show that the change in electrical conductivity is bolometric (caused by heating of the SWNT network). Electron-phonon interactions lead to ultrafast relaxation of the photoexcited carriers and the energy of the incident infrared radiation is efficiently transferred to the crystal lattice. The photoinduced changes in resistance occur as result of temperature changes rather than by photoexcited holes and electrons and we consider the implications of this result for the band and exciton models in carbon nanotubes. We show that the infrared photoresponse of suspended SWNT films is sufficiently high that they may function as the sensitive element of an infrared bolometric detector. M.E.Itkis, F.Borondics, A.Yu, R.C.Haddon, Science 312, 413 (2006)

1Supported by DOD/DARPA/DMEA grants DMEA90-02-2-0216, H94003-04-2-0404, H94003-05-2-0504, FB acknowledges support from a Fulbright Association. FB present address: MTA SzFKI, Budapest, I 1525, Hungary.

Monday, March 5, 2007 11:15AM - 2:03PM
Session B39 FIAP DMP: Focus Session: Materials and Applications for Solar Energy I Colorado Convention Center 502
11:15AM B39.00001 Multiple Exciton Generation for Highly Efficient Solar Cells1, ARTHUR NOZIK, National Renewable Energy Laboratory — In order to utilize solar power for the production of electricity and fuel on a massive scale, it will be necessary to develop solar photon conversion systems that have an appropriate combination of high efficiency and low capital cost ($/m^2$). One new potential approach to high solar cell efficiency is to utilize the unique properties of semiconductor quantum dot nanostructures to control the relaxation dynamics of photogenerated carriers to produce either enhanced photocurrent through efficient multiple exciton generation (MEG) or enhanced photopotential through hot electron transport and transfer processes. To achieve these desirable effects it is necessary to understand and control the dynamics of electron relaxation, cooling, multiple exciton generation, transport, and interfacial electron transfer of the photogenerated carriers with fs to ns time resolution. We have been studying these fundamental dynamics in bulk and nanoscale semiconductors (quantum dots, quantum wires, and quantum wells) using femtosecond transient absorption, photoluminescence, and THz spectroscopy. This work will be summarized and recent advances in creating multiple excitons from a single photon will be discussed, including a unique model to explain efficient MEG based on the coherent superposition of multiple excitonic states. Various possible configurations for quantum dot solar cells that could produce ultra-high conversion efficiencies for the production of electricity, as well as for producing solar fuels (for example, hydrogen from water splitting), will be discussed, along with associated thermodynamic calculations that show the increase in the maximum theoretical gain in solar photon conversion efficiency for both electricity and fuel production.

1Work funded by the U.S. DOE Office of Basic Energy Sciences

11:51AM B39.00002 Optical properties of II-VI structures for solar energy utilization, JOSHUA SCHRIER, DENIS DEMCHENKO, LIN-WANG WANG, Lawrence Berkeley National Laboratory — Although II-VI semiconductor materials are abundant, stable, and have direct band gaps, the band gaps are too large for optimal photovoltaic efficiency. However, staggered band alignments of pairs of these materials, and also the formation of intermediate impurity levels in the band gap (which has been demonstrated to increase the efficiency as compared to both single-junction devices), could be utilized to improve the suitability of these materials for solar energy utilization. Previous theoretical studies of these materials are limited, due to the well-known band gap understimation by density-functional theory. To calculate the absorption spectra, we utilize a band-corrected plane-wave pseudopotential approach, which gives agreements of within 0.1 eV of the bulk optical gaps values. In this talk, I will present our work on predicting the optical properties of ZnO/ZnS and ZnO/ZnTe heterostructures, nanostructures, and alloys. This work was supported by U.S. Department of Energy under Contract No.DE-AC02-05CH11231 and used the resources of the National Energy Research Scientific Computing Center.

12:03PM B39.00003 Local Structures Around S in CdS:O Thin Films Photovoltaic Materials Probed by S K-edge X-ray Absorption Fine Structures1, Y. L. SOO, W. H. SUN, S. C. WENG, Y. S. LIN, S. L. CHANG, National Tsing Hua University, Taiwan, L. Y. JANG, NSRRC, Taiwan, X. WU, Y. YAN, NREL — Local Structures around S in thin films of CdS:O have been investigated using EXAFS and NEXAFS techniques at the S K absorption edge. Our S K-edge EXAFS results clearly indicate the presence of S-O bonds that coexist with S-Cd bonds in the oxygen-containing samples. The S K-edge NEXAFS data further identify SO$_3$ and SO$_4$ complexes in the samples. As indicated by our previous results on Cd K-edge EXAFS, Cd atoms are predominantly bonded with S. These x-ray results demonstrate that the oxygen atoms actually combine with S to form SO$_3$ and SO$_4$ complexes instead of being incorporated into the CdS host. In combination with the evidence of nanodendrites revealed by TEM, our results suggest that oxygen-free CdS nanocrystals are formed in the films due to the O content. The bandgap of the samples is therefore found to increase with O concentration as opposed to the bandgap decrease for O doping expected in the band anticrossing model. 2The present research has been supported by NSC in Taiwan under project number 95-2112-M-007-014- and by NSF/ONR in the US under Award No. 0223848.

12:15PM B39.00004 P-type InGaN alloys, D. M. YAMAGUCHI, R. E. JONES, N. R. MILLER, E. E. HALLER, U. C. Berkeley, Berkeley CA, 94720...
1:15PM B39.00007 Novel photophysics and tandem device designs for solar hydrogen production, JUSTIN JOHNSON, MATT LAW, NATHAN NEALE, ARTHUR FRANK, JOSEF MICHL, ARTHUR NOZIK, National Renewable Energy Lab — Solar hydrogen production by water photolysis could provide a means for generating large quantities of clean, transportable fuel cheaply and efficiently for a wide variety of energy uses. Previous schemes of solar hydrogen production have not resulted in a suitable combination of high efficiency, low cost, and good long-term stability to meet requirements for their practical utilization in large-scale energy production. Revolutionary technologies and application of novel photophysical concepts represent a pathway toward overcoming current barriers and achieving an entirely practical method for producing solar fuels. One such concept is the utilization of tandem device designs, which allow for the incorporation of visible/near-IR absorbing materials into the device, thus increasing solar flux harvesting. Moreover, including molecules capable of charge multiplication (multiple electrons/holes per single photon) holds the prospect for additional gains in solar-to-hydrogen efficiencies. Current progress as well as future challenges for developing such devices will be discussed, including simulations, fundamental spectroscopic experiments, and device design and construction.

1:27PM B39.00008 Optimization of Nanostructured ZnO / Conjugated Polymer Photovoltaic Devices, DANA OLSON1, YUN-JU LEE, ERICK SPOERKE, DARREN DUNPHY, JAMES VOIGHT, JULIA HSU, Sandia National Labs, MATTHEW WHITE, Univ. of Colorado, SEAN SHAHEEN, DAVID GINLEY, National Renewable Energy Lab — Nanostructured oxide semiconductor / conjugated polymer composites are promising systems for low cost photovoltaic devices. The use of nanostructures increases the heterojunction areas, resulting in more effective capturing of photogenerated charges. We have fabricated arrays of ZnO nanorods by low-temperature solution growth on patterned ITO substrates. The dense ZnO nanorod arrays are subsequently infiltrated with poly(3-hexylthiophene) (P3HT), and the devices are completed by depositing Ag top electrodes. Depending on the seeding conditions, we can control the alignment of ZnO nanorods on ITO: ordered (aligned perpendicular to the substrate) versus disordered. We will study the effects of nanorod array morphology and growth chemistry, as well as processing conditions used to infiltrate P3HT into the ZnO nanorod arrays. We will also examine surface treatment and modification of ZnO prior to polymer infiltration to enhance electron transfer efficiency at the ZnO/P3HT heterojunctions. Finally, these results are correlated with the device data to observe the effects of ZnO nanorod ordering, interfacial treatment, and the infiltration process on the device performance.1

1:39PM B39.00009 Theoretical Insights on Interfacial Charge Transfer across the P3HT/Fullerene Photovoltaic Heterojunction from ab Initio Calculations, YOSUKE KANAI, JEFFREY C. GROSSMAN, Berkeley Nanosciences and Nanoengineering Institute (BNNI), University of California, Berkeley — Within the current effort to develop more efficient and less expensive solar cell devices, the polymer/fullerene photovoltaic (PV) structure is considered to be very promising. The crucial component of such a PV structure is the nano-scale heterojunction interface of the polymer and the fullerene. This interface must facilitate the dissociation of the exciton which is formed in the polymer, so that separated charges can be generated across the interface. Our current understanding of the charge separation mechanism at an atomicistic level is rather limited, slowing the progress in the structural design of the heterojunction interface. We employ ab initio calculations to investigate and characterize the charge transfer state which is responsible for the charge separation process. Our results elucidate several important phenomena regarding this mechanism, which lies at the heart of higher power conversion efficiency in polymeric solar cell devices.

1:51PM B39.00010 Hybrid Tandem Solar Cells: CIGS/DSC with Carbon Nanotube Interlayer, ANVAR ZAKHIDOV, UTD-Nanotech Institute, WILLIAM SHAFARMAN, Institute Energy Conversion, University of Delaware, MEI ZHANG, UTD-NanoTech Institute, SHAOLI FANG, UTD-Nanotech Institute, RAY BAUGHMAN, UTD-Nanotech Institute, TX75070 — Multi-junction solar cells enable harvesting of wider regions of the solar radiation spectrum leading thereby to increased overall efficiencies. We present here a first study of a hybrid monolithic structure composed of dye sensitized solar cells (DSCs) with thin film inorganic CIGS. We have created several architectures of monolithic multi-junction cells and address fundamental connectivity issues by using sheets of strong, transparent carbon nanotubes (T-CNTs) recently produced at UTD [1] as a uniform interlayer platform. Free-standing T-CNT networks can be laminated onto any surface and their advantages as transparent interlayers in tandems is shown here for a tandem in which a un-finished CIGS (top ITO is absent) is coated by T-CNTs. Such CIGS with T-CNT shows Voc≈0.6 V and Isc~10 mA/cm2. It has been combined with DSC playing role of a photoactive counter-electrode, with iodine based electrolyte and Ru-dye on TiO2 mesoscopic electrode. The tandem demonstrated Voc= 0.82 V, which is higher than Voc of our sole DSC-CNT and Isc=1mA/cm2, smaller than photocurrent of single DSC due to unbalanced current. The physics of processes of charge recombination in hybrid tandems is discussed.[1] M. Zhang, S. Fang, A. Zakhidov, S. B. Lee, A. Aliev, R.H. Baughman, Science, 309,(2005) 1215

Monday, March 5, 2007 11:15AM - 1:51PM – Session B42 DMP: Focus Session: Kinetics of Self-Assembly at Surfaces Colorado Convention Center

11:15AM B42.00001 Theory of kinetics of surface evolution: simulations, Langevin, and Fokker-Planck approach, ALBERTO PIMPINELLI, Université Clermont-2 & University of Maryland — The study of the the time evolution of morphological features at crystal surfaces has become a topic of great importance, motivated in part by the need of achieving controlled fabrication of nanostructures, and in part by the fundamental statistical mechanics questions that it raises. For the evolution of nanostructure, the control of step dynamics is critical, since the steps are the fundamental building blocks of crystalline surfaces. Kinetic Monte Carlo (KMC) simulations, coupled to Langevin-type analysis of the scaling properties of step dynamics is a powerful tool for assessing the universal features of surface fluctuations close and far from equilibrium. We discuss the results of KMC simulations of unstable growth of vicinal surfaces, that exhibit anomalous scaling exponents as well as multiscaling. We also discuss a tentative interpretation of the numerics within the Langevin approach, as well as the usefulness of the results in interpreting experimental data. Other theoretical tools, such as the spacing distribution of the eigenvalues of random matrices have been employed, e.g. for investigating the evolution of the terrace width distribution (TWD) on stepped surfaces. We discuss KMC simulations of the relaxation of non equilibrium surface structures towards the equilibrium state. Our results show that relaxation far from equilibrium may be driven by microscopic processes, such as detachment of three-bonded atoms, that differ from those that drive step fluctuations close to equilibrium. Applications of the formalism to out-of-equilibrium states, such as step flow growth, are discussed.1

1 A.P. acknowledges support from the Kavli Foundation and the CNRS
11:51AM B42.00002 Strain induced metastability in the shape evolution of self-assembled nanoislands on Si(111): real-time electron microscopy observations and numerical simulations .

NIKHIL MEDHEKAR, VIVEK SHENOY, Division of Engineering, Brown University, JAMES HANNON, IBM Research Division, T. J. Watson Research Center — We present real-time low-Energy Electron Microscopy (LEEM) observations of the growth and equilibrium shapes of (7x7) reconstructed domains on (1x1) reconstructed Si(111) surface which show several intriguing features in its shape evolution due to strain mediated interactions. We find that the shapes of large domains are fundamentally different from the compact shapes of smaller domains. In contrast, large islands show more lamellated shapes resembling branched pine-tree when grown at faster rate and connected-triangles morphology when growth is near equilibrium. Using a phase-field model, we show that the key to understanding this behavior is the strain induced metastability of domain shapes that are trapped in the local minima of the complex energy landscape. The consideration of growth shapes that show spontaneous formation of side branches is necessary to establish the presence of unstable orientations and thus, our work shows that in estimating the thermodynamic and kinetic parameters, the conclusions solely drawn based on the analysis of equilibrium shapes can be erroneous.

12:03PM B42.00003 Atom-Scale Mechanisms for Unstable Growth on Patterned GaAs(001)

TABBASSOM TADAYON-ESLAMI, HUNG-CHIH KAN, University of Maryland, LYNN CALHOUN, Laboratory for Physical Sciences, RAY PHANEUF, University of Maryland — Molecular beam epitaxy on patterned GaAs(001) under standard conditions of temperature (~600 °C), rate (~0.3 nm/s) and flux ratio (As2/Ga~10:1) leads to a transient instability toward perturbation of the flat surface [1]. Lowering the temperature through approximately 540°C, roughly coincident with the preroughening temperature changes the mode of this instability [2]; however, as we show in this talk, observations of the As2 flux dependence rule out both preroughening and a reconstructive phase transition as driving the growth mode change. Instead, we find evidence that the change in unstable growth mode can be explained by a competition between decreased adatom collection rate on small terraces and a small anisotropic multi-step Ehrlich-Schwoebel barrier. We relate these effects to the up-down symmetry breaking term which commonly appears in continuum equations for growth. [1] H.-C. Kan, S. Shah, T. Tadayon-Eslami and R.J. Phaneuf, Phys. Rev. Lett., 92, 146101 (2004). [2] T. Tadayon-Eslami, H.-C. Kan, L. C. Calhoun and R. J. Phaneuf, Phys. Rev. Lett., 97, 126101 (2006).

12:15PM B42.00004 Growth Kinetics of Ge Quantum-dots Formed by Thermal Oxidation of Si1-xGex-on-insulator and Its Related Physical/Electrical Properties

PEI-WEN LI, WAI-TING LAI, DAVID MING-TING KUO, National Central University — Using thermal oxidation of SiGe-on-insulator (SGOI) for forming Ge quantum dots (QDs) embedded in SiO2, we have investigated possible factors that would affect the nature of Ge QDs, such as size, density, and even the position. The positions of the Ge QDs are found to be dependent on oxidation condition, Ge content in SiGe, layer thickness and geometric patterns of SGOI structures. Tiny and dense (3 nm/2.8×1012 cm−2) QDs could be formed by oxidizing a SGOI wafer, which is well suitable for nonvolatile memory applications. While a single QD (10 nm) would be formed and simultaneously self-aligned to electrodes by SiO2 barriers if oxidation is performed to a SGOI nanowire, which is highly demanded for successful single-electron devices. Photo-excitation effect on carrier transport through Ge-QD/SiO2 system is studied via Ge-tunneling diodes. Under optical pumping, the tunneling current displays additional oscillatory peaks and enhanced negative differential conductance, indicating holes created in the QD by optical pumping lead to additional channels via the electron-hole interaction for electron tunneling.

12:27PM B42.00005 Multiscale simulations of self-assembly of CdTe nanoparticles into sheets

ZHENLI ZHANG, ZHIYONG TANG, NICOLAS KOTOV, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109, USA — By controlling the organic stabilizers on the surfaces of CdTe nanodots, these particles are found in experiments to self-assemble into one-dimensional wires and two-dimensional sheets[1,2]. To explore the underlying mechanisms for the two processes we perform simulations on multiple scales ranging from quantum mechanics to mesoscale stochastic simulations[2,3]. The simulations and corresponding energy analysis demonstrate that a delicate balance of anisotropic forces between nanoparticles is responsible for the different nanostructures they form. In particular, we show how nanoparticle shape, directional hydrophobic attraction, and electrostatic interactions determine the anisotropy of the interaction and final self-assembled structures. [1] Tang ZY, Kotov NA, Giersig M, Science, 297, 237-240, 2002. [2] Tang ZY, Zhang ZL, Wang Y, Glotzer SC and Kotov NA, Science, 314, 274-278, 2006. [3] Zhang ZL, Tang ZY, Kotov NA and Glotzer SC, preprint.

12:39PM B42.00006 Charging in CdSe nanocrystals and mechanistic elucidation of the electrophoretic deposition of nanocrystal films

SHENGGUO JIA, SARBABJIT BANERJEE, IRVING HERMAN, Materials Research Science and Engineering Center, Columbia University — The charge on nanocrystals is not only used to stabilize the colloidal systems but also to assemble these materials into novel films and superlattices. Here, we propose a model for charging in nanocrystals involving the dissociation of ligand molecules from specific surface sites. We also develop a mechanistic model to explain the electrophoretic deposition of nanocrystal films based on electrophoretic mobility measurements, photoluminescence from nanocrystal solutions and films, and observations from deposition experiments. Even though equally thick nanocrystal films are obtained on both negative and positive electrodes, the numbers of positive and negative nanocrystals are not equal in solution. After appropriate reprecipitation cycles, the nanocrystals are "sticky" enough to be deposited on the electrodes and nanocrystal films can be formed by electrophoresis. The limiting factor for the maximum thickness to which the films can be grown is the concentration of the minority charged crystals (negatively charged nanocrystals in this case). The charge on the nanocrystal surfaces can be adjusted by the addition of ligands. This work was supported primarily by the MRSEC Program of the NSF under Award No. DMR-0213574 and by NYSTAR.

12:51PM B42.00007 Phase Field Crystal Modeling of Island Formation and Dislocation Nucleation During Strained Film Growth

ZHI-FENG HUANG, Dept. of Physics and Astronomy, Wayne State University, KEN ELDER, Dept. of Physics, Oakland University — We study the process of nanostructure self assembly during epitaxial growth of strained solid films through the use of the phase field crystal model. The model is derived from density functional theory and incorporates anisotropy, elasticity and plastic deformations on atomic length and diffusive time scales. We particularly address the formation and evolution of islands/mounds in strained thin films following an initial morphological instability and the nucleation and climb of misfit dislocations. The relation between film structural properties and materials and growth conditions are also discussed.
1:03PM B42.00008 An Investigation into InAs/GaAs Thin Film Growth1. MARIA MIGNOGNA, KRISTEN FICHTHORN, Penn State University — Quantum dots self-assemble due to Stranski-Krastinov growth in heteroepitaxial systems with a lattice mismatch above 2%, for example in the deposition of InAs on GaAs (001). However, there are many questions left unanswered about quantum dot growth, such as the role of strain in the wetting layer. Simulation techniques such as molecular dynamics (MD) can provide insight at the atomic scale. An empirical potential to study this system has recently been developed [1]. Using NPT MD, we studied the thermal properties and melting of bulk GaAs, as well as the stability of the GaAs(001)/32(2x4) reconstruction against melting. To probe diffusion and the preferred Ga-atom binding sites, we calculated the minimum potential-energy surface for a gallium atom on the GaAs (001)32(2x4) reconstruction. We also evaluated various diffusion pathways and energy barriers using the nudged elastic-band method. The potential captures the location and energy of the deepest binding minimum as compared to DFT values and also achieves good agreement for the diffusion barriers. We used accelerated MD simulations to obtain diffusion coefficients as a function of temperature and these compare favorably to previous results from experiment and DFT. [1] T. Hammerschmidt, PhD Thesis (2006)

1Supported by NSF DGE 9987598

1:15PM B42.00009 Nanocrystal Formation in Ion-Beam Synthesized GaAs:N and InAs:N, A. WOOD, Dept. of Physics, W. YE, X. WENG, P.T. WANG, R.S. GOLDMAN, Dept. of Mat. Science & Engin., Univ. of Michigan, Y.Q. WANG, Mat. & Tech. Div., Los Alamos Natl., Lab — Ion-implantation followed by thermal annealing offers a unique approach to custom tailoring of semiconductor nanocomposites. For N ion-implanted GaAs (GaAs:N), an amorphous layer with crystalline GaAs remnants is often observed. Subsequent furnace or rapid-thermal annealing (RTA) leads to the formation of zincblende (ZB) GaN nanocrystals [1], which transform to wurtzite (WZ) following extended furnace annealing [2]. For N ion-implanted InAs (InAs:N), nanocrystal formation and evolution has not been previously reported. We are studying the formation and evolution of GaAs:N and InAs:N nanocomposites, synthesized using 100keV ion-implantation with a dose of 5x1012 cm−2, at 300C and 77K. In all cases, the as-implanted structures are primarily amorphous. For GaAs:N, RTA up to 625C leads to an amorphous layer with crystalline GaAs remnants, while RTA in the range 675-700C results in both ZB and WZ nanocrystal. For InAs:N, 500C RTA leads to the formation of ZB InN-rich and InAs-rich nanocrystals, with amorphous matrices and domains. We will discuss the role of crystalline remnants in the nucleation and growth of ZB nanocrystals, and the mechanisms of the ZB-WZ transformation.

Aarhus Universitet, Aarhus, Denmark, U. GERSTMANN, Universite Pierre et Marie Curie, Paris, France — Donors in strained Si layers have been proposed for quantum dots and qubits [1]. Oscillations in strained layers which would otherwise limit the exchange interaction of neighboring qubits. Via electrically detected magnetic resonance, we have measured the hyperfine interaction of phosphorus donors in fully strained Si thin films grown on virtual Si(001) and SiGe substrates with x ≤ 0.3, extending the regime investigated earlier by a factor of 20 to higher strains. For highly strained epilayers, hyperfine interactions as low as 0.8 mT are observed [1]. Within a Green’s function approach, density functional theory shows that the additional reduction is caused by the volume increase of the unit cell and a relaxation of the Si ligands of the donor. [1] H. Hübli et al., Phys. Rev. Lett. 97, 166402 (2006).

1:27PM B42.00010 Dual-surfactant effect on enhancing Zn-Doping of GaP1. JUNYI ZHU, GERALD STRINGFELLOW, FENG LIAO — We report first-principles calculations demonstrating a dual-surfactant effect of Sb and H on enhancing Zn-doping in vapor phase epitaxially grown GaP thin films. The combined effects of Sb and H lower significantly the doping energy of Zn in GaP, while neither Sb nor H can work alone as effectively. The role of H is to provide the extra electron accommodating the p-type dopant incorporation to satisfy the electron counting rule. Our finding has an important general implication that p-type doping in III-V thin films can be achieved by chemical deposition with H, but difficult by physical deposition without H.

1This work is supported by the Department of Energy, Division of Basic Energy Sciences.

1:39PM B42.00011 Design Principles Incorporating Surface Dynamics for Creating Ordered Organic Nanostructures on Si and SiC Dimerized Surfaces via Car-Parrinello Molecular Dynamics, ROBIN HAYES, MARK TUCKERMAN, New York University — Self-assembled organic nanostructures on Si-type semiconducting surfaces promise to impact nanoelectronics, sensors, and nanolithography. Experimentalists have long exploited cycloaddition reactions between small conjugated molecules and Si surface dimers, but with limited success in creating well-ordered structures. Cycloaddition of 1,3-cyclohexadiene (CHD) to the Si(100)-2x1 surface provides a rich test case to explore the role surface dynamics play in the product distribution with thermodynamic predictions. Car-Parrinello molecular dynamic simulations reveal that the local surface environment, including dimer tilt angle and dimer flipping, matters. CHD often travels over several dimers before forming an adduct by a two step process. First the C=C reacts with a “down” Si. The intermediate can persist for over 4 ps and can cause nearby dimers to flip, allowing CHD to complete the reaction with any of the adjacent Si. Thereby, accounting for most of the experimental product distribution. Previously formed adducts protect Si within a 5.5 Å radius and direct the surface exploration of unbound CHD. These principles are tested on reactions between 1,3-CHD and the closely related 3C-SiC(001)-3x2 surface.

Monday, March 5, 2007 11:15AM - 2:15PM –
Session B43 DMP: Focus Session: Materials for Quantum Information Processing I Colorado Convention Center 506

11:15AM B43.00001 Sputtered Gold as an Effective Schottky Gate for Strained Si/SiGe Nanostructures, GAVIN SCOTT, MING XIAO, UCLA Dept of Physics, ED CROKE, HRL Laboratories, ELI YABLONOVITCH, UCLA Dept of Electrical Engineering, HONGWEN JIANG, UCLA Dept of Physics — Metalization of Schottky gate so-called low leakage contacts for Au on strained Si/SiGe heterojunctions enables the depletion of the two dimensional electron gas (2DEG) at a relatively small voltage while maintaining an extremely low level of leakage current. A fabrication process has been developed to enable the formation of sub-micron Au electrodes sputtered onto Si/SiGe without the need of a wetting layer.

11:27AM B43.00002 Phosphorus Donors in Highly Strained Silicon1, M. S. BRANDT, H. HUEBL, A. R. STEGNER, M. STUTZMANN, Walter Schottky Institut, Garching, Germany, G. VOOG, F. BENSCH, Fraunhofer IZM, Muenchen, Germany, E. RAULS, Aarhus Universitet, Aarhus, Denmark, U. GERSTMANN, Université Pierre et Marie Curie, Paris, France — Donors in strained Si layers have been proposed for quantum computing applications. The lifting of the six-fold valley degeneracy, characteristic for unstrained Si, leads to a suppression of the Kohn-Luttinger oscillations in strained layers which would otherwise limit the exchange interaction of neighboring qubits. Via electrically detected magnetic resonance, we have determined the hyperfine interaction of phosphorus donors in fully strained Si thin films grown on virtual Si1-xGe, substrates with x ≤ 0.3, extending the regime investigated earlier by a factor of 20 to higher strains. For highly strained epilayers, hyperfine interactions as low as 0.8 mT are observed [1], significantly below the limit predicted by valley repopulation. Within a Green’s function approach, density functional theory shows that the additional reduction is caused by the volume increase of the unit cell and a relaxation of the Si ligands of the donor. [1] H. Hübli et al., Phys. Rev. Lett. 97, 166402 (2006).

1Supported by DFG (SFB 631)
11:39AM B43.00003 Process integration and electron spin coherence of donor atom implants in silicon, T. SCHENKEL, Lawrence Berkeley Laboratory, A. PERSAUD, LBNL, A. M. TYRSHSHKIN, S. A. LYON, Princeton University, J. BOKOR, C. C. LO, R. DESOUZA, UC Berkeley, I. CHAKAROV, Silvaco Internat. — We implanted low doses (2 to 4 x 10^{12} m^{-2}) of P, Sb, and Bi ions into isotopically enriched silicon (28-Si) and characterized diffusion, electrical activation and electron spin coherence after rapid thermal annealing. Phosphorus and bismuth both exhibit enhanced segregation to an imperfect Si/SiO2 interface, while dopant movement is suppressed for antimony ions. Pulsed electron spin resonance shows that spin echo decay is sensitive to the dopant depths, and the interface quality. At 5.2 K, a spin de-coherence time, T2, of 0.3 ms is found for Sb profiles peaking 50 nm below a Si/SiO2 interface, increasing to 0.75 ms when the surface is passivated with hydrogen. These measurements provide benchmark data for the development of devices in which quantum information is encoded in donor electron spins [1]. [1] T. Schenkel, et al., Appl. Phys. Lett. 88, 112101 (2006).

11:51AM B43.00004 Double donors in Si quantum computer architecture, MARIA J. CALDERON, Condensed Matter Theory Center, University of Maryland, BELITA KOILLER, Instituto de Fisica, Universidade Federal do Rio de Janeiro, Brazil, SANKAR DAS SARMA, Condensed Matter Theory Center, University of Maryland — We discuss the possibility of performing single spin measurements in Si-based quantum computers through electric field control of electrons bound to double donors near a barrier interface[1]. In particular, we investigate the feasibility of shuttling donor-bound electrons between the double donor impurity in the bulk and the Si/SiO2 interface by tuning an external electric field. We find that both the required electric fields and the tunneling times involved are probably too large for practical implementations. We also investigate operations with double donors in their first excited state: In this case ionization fields are smaller and tunneling times are faster, as required in spin-to-charge conversion measurements. This work is supported by LPS and NSF [1] M.J. Calderon, B. Koiller, and S. Das Sarma, cond- mat/0610089.

12:03PM B43.00005 Electric-field driven donor-based charge qubits in semiconductors, BELITA KOILLER, Instituto de Fisica, UFRJ, Rio de Janeiro, Brazil, XUEDONG HU, University at Buffalo, SUNY, Buffalo, NY, SANKAR DAS SARMA, CMTC, Department of Physics, UMD, Maryland — We theoretically investigate donor-based charge qubit operation driven by external electric fields [1]. We consider initially a single electron bound to a shallow-donor pair in GaAs: This system allows the basic physics of the system to be presented. In the case of Si, heteropolar configurations such as P-Sb+ pairs are also considered. For both homopolar and heteropolar pairs, the multivalley conduction band structure of Si leads to short-period oscillations of the tunnel-coupling strength as a function of the relative position of the donors. However, for any fixed donor configuration, the response of the bound electron to a uniform electric field in Si is qualitatively very similar to the GaAs case, with no valley quantum interference-related effects, leading to the conclusion that valley interference does not prevent the coherent manipulation of donor-based charge qubits by external electric fields. We also discuss the effect of perturbations due to additional distant donors. [1] B. Koiller, X. Hu, and S. Das Sarma, Phys. Rev. B 73, 045319 (2006)

12:15PM B43.00006 Suppressing anisotropic hyperfine induced electron spin echo modulations in Si:P, WAYNE WITZEL, University of Maryland, XUEDONG HU, University at Buffalo, SANKAR DAS SARMA, University of Maryland — In previous work [1] our theory of spectral diffusion (SD) agrees well with electron spin echo decay measurements in Si:P. In addition to SD decay, these experiments show strong electron spin echo envelope modulations (ESEEM) that significantly reduce spin coherence at short echo times relative to SD decay. Strong demands imposed by fault tolerant quantum computing require suppression (or exploitation) of this effect in order to realize spin-based quantum computation in Si:P systems. It is known that these modulations, caused by anisotropic hyperfine interactions with 29Si nuclei, can be suppressed via isotopic purification, or by applying a strong, ~ 10 T magnetic field. Our insights lead to an alternative approach that eliminates predominant modulations at modest magnetic fields (~ 1 T) with little need for isotopic purification. Our calculations are in remarkable agreement with experiment, showing good theoretical understanding of refocused electron spin coherence in Si:P systems.

1 Supported by ARO and LPS
3 A.M. Tyrshshkin, et al., cond-mat/0512705.

12:27PM B43.00007 Electron transport through STM-patterned dopants in silicon, MICHELLE SIMMONS, University of New South Wales — The recent adaptation of scanning probe systems for nanoscale device fabrication has opened the door to creating electronic devices in silicon with single atom precision. Using a combination of STM lithography and molecular beam epitaxy we show how we can pattern planar, highly doped P layers in silicon down to the atomic-scale and electrically contact them outside the microscope environment. Having developed this technology we demonstrate conduction through silicon nanowires with widths down to 8nm that still exhibit ohmic conduction with resistivities as low as 3x10^{-11}m. We present a study to determine what ultimately limits conduction in these systems as well as studies of tunnel gaps as charge detectors, ordered dopant arrays and transport through silicon dots. We will present an overview of devices that have been made with this technology and highlight some of the challenges to achieving truly atomically precise devices such as a silicon based quantum computer.

3 MYS acknowledges the Australian Research Council, the NSA and the SRC for financial support.

1:03PM B43.00008 Electron Spin Resonance on Arrays of Etched Quantum Dots in 28Si:SiGe, JIANHUA HE, A. M. TYRSHSHKIN, S. A. LYON, Princeton University, D. E. SAVAGE, M. A. ERIKKSON, University of Wisconsin-Madison — Relaxation times of 2-dimensional electrons in Si quantum wells (QW) in Si:SiGe heterostructures are found to be shorter than the extremely long relaxation of 3-dimensionally confined donor-bound electrons in Si. Confining the electrons into quantum dots (QD) could suppress the Dyakonov-Perel spin relaxation due to fluctuating Rashba fields, and thus lead to long relaxation times for electrons in QDs. We have developed a reliable, low-defect density process to pattern large area 2D arrays (several cm²) of nominally 100nm dots with a 200nm pitch in a CVD grown 28Si:SiGe quantum well. The process involves nanoimprinting, reactive ion etching and wet etching. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) imaging has been used to characterize the etch depth (various depths up to 60nm) and uniformity. After etching we find an electron spin resonance signal with a g-factor of 1.9998, which is considerably shifted from that of the unetched QW (2.003). This line exhibits anisotropies of its g-factor and linewidth that are similar to those of 2D electrons, as might be expected for large, flat QDs. This new line is also broader (420 mG) than that from the unetched QW (90 mG) which could result from an inhomogeneity in dot sizes.
1:15PM B43.00009 Electron Spin Resonance of Electrons in a Large-Area Silicon MOSFET. SHYAM SHANKAR, A. M. TYRYSHKIN, SUSHOBHAN AVASTHI, S. A. LYON, Dept. of Electrical Engineering, Princeton University — Spins of electrons in two-dimensional (2D) semiconductor heterostructures are considered as qubit candidates for quantum information processing. Electron spin resonance (ESR) of silicon MOSFETs can be useful in characterizing electrons in 2D structures, but previous attempts have been inconclusive. To have sufficient signal for ESR measurements, a large area n-channel silicon FET with a 100nm thick oxide was made using standard processing techniques. Two ESR signals were seen at temperatures below 20K with a gate bias above the threshold voltage of 0.9V. A weak signal with a linewidth of 1G, at g=1.9988(1) may be similar to one observed by Wallace et al., in the Silsbee [PRB 1991 43 9941]. This signal shows a noticeable increase in g-factor from 1.999 at 1V to 2.000 at 1.7V gate bias and a corresponding decrease in linewidth from 500mG to 400mG. A small g-factor and linewidth change is also observed when the FET is rotated with respect to the applied magnetic field. The signal intensity shows non-Curie temperature behavior below 10K. Such a signal, possibly from conducition electrons or electrons in shallow traps, has not been reported before and is being further investigated.

1:27PM B43.00010 Electrically Detected Magnetic Resonance of Slow Donors in Accumulation Layer MOSFETs. CHEUK CHI LO, J. BOKOR, University of California, Berkeley, T. SCHENKEL, R. DE SOUSA, Lawrence Berkeley National Labs, JIANHUA HE, G. SABOURET, S. SHANKAR, F. R. BRADBURY, A. M. TYRYSHKIN, S. A. LYON, Princeton University — The ability to read out the spin state of a single donor-bound electron is an essential, but not yet demonstrated, capability for building a quantum computer processor using the spins of electrons bound to Si donors as the qubits. We present measurements of the spins of ensembles of shallow donors embedded in the channel of a MOSFET. Our approach is based on spin-dependent transport arising from the fact that the scattering cross-section of conduction electrons with donor electrons is much greater than the spins of donors. We report the isolation of a single electron in a Si QD using a fabrication technique that incorporates the standard Al/SiO2/Si system with an enhancement mode lateral QDs in the GaAs/AlGaAs single electron transistors (SETs) have been intensively investigated. In contrast, Si provides a number of advantages, including the two Zeeman states of an electron spin in a quantum dot (QD) provide a promising candidate for a qubit. Spins in lateral QDs in the GaAs/AlGaAs single electron transistors (SETs) have been intensively investigated. In contrast, Si provides a number of advantages, including long spin coherence time, large g-factor, and small spin-orbit coupling effect. We have demonstrated Si SET in the few electron regime. In this talk, we will report the isolation of a single electron in a Si QD using a fabrication technique that incorporates the standard Al/SiO2/Si system with an enhancement mode SET structure. Our SET is built in highly resistive Si substrates with bilayer gates. The high purity Si minimizes the potential disorder from impurities. The top gate induces 2D electrons, and several side gates help define the tunneling barriers, fine tune the shape of the QD, and control the number of electrons in it. We will discuss the operating principle, computer simulation, and low temperature transport data. *APPLIED PHYSICS LETTERS 89, 073106 (2006)

2:03PM B43.00013 Enhancement mode single electron transistor in pure silicon, BINHUI HU, C.H. YANG, Department of Electrical and Computer Engineering, University of Maryland, College Park, MD 20742. G.M. JONES, M.J. YANG, Naval Research Laboratory, Washington DC 20375. — Solid state implementations of lateral qubits offer the advantage of being scalable and can be easily integrated by existing mainstream IC technologies. In addition, the two Zeeman states of an electron spin in a quantum dot (QD) provide a promising candidate for a qubit. Spins in lateral QDs in the GaAs/AlGaAs single electron transistors (SETs) have been intensively investigated. In contrast, Si provides a number of advantages, including long spin coherence time, large g-factor, and small spin-orbit coupling effect. We have demonstrated Si SET in the few electron regime. In this talk, we will report the isolation of a single electron in a Si QD using a fabrication technique that incorporates the standard Al/SiO2/Si system with an enhancement mode SET structure. Our SET is built in highly resistive Si substrates with bilayer gates. The high purity Si minimizes the potential disorder from impurities. The top gate induces 2D electrons, and several side gates help define the tunneling barriers, fine tune the shape of the QD, and control the number of electrons in it. We will discuss the operating principle, computer simulation, and low temperature transport data. *APPLIED PHYSICS LETTERS 89, 073106 (2006)

1:15AM B44.00001 Conductance of Single Molecule Junctions: Dependence on Structure and Conformation. LATHA VENKATARAMAN, Columbia University — We recently demonstrated that the conductance of single molecule junctions formed by breaking Au point contacts in an environment of molecules with amine linkages can be measured reliably and reproducibly. We have now studied junctions formed by approximately 30 different amine terminated molecules, allowing systematic study of the correlation between molecular properties and single molecule junction conductance. This talk will focus on the relation between molecular conductance and molecule conformation for the simple case of a biphenyl, two benzene rings linked together by a single C-C bond. Our results from a series of seven biphenyl derivatives show that the molecular junction conductance depends on the twist angle. Specifically, we find that the planar molecule has the highest conductance, and the conductance for the series decreases with increasing twist angle, consistent with a cosine squared relation predicted theoretically. 1. L. Venkataraman, J.E. Klare, I.W. Tam, C. Nuckolls, M.S. Hybertsen and M. Steigerwald, Nano Letters, vol. 5, pp. 458-462, 2006. 2. L. Venkataraman, J.E. Klare, C. Nuckolls, M.S. Hybertsen and M. Steigerwald, Nature, vol. 442, pp. 904-907, 2006.

11:15AM B44.00001 Conductance of Single Molecule Junctions: Dependence on Structure and Conformation. LATHA VENKATARAMAN, Columbia University — We recently demonstrated that the conductance of single molecule junctions formed by breaking Au point contacts in an environment of molecules with amine linkages can be measured reliably and reproducibly. We have now studied junctions formed by approximately 30 different amine terminated molecules, allowing systematic study of the correlation between molecular properties and single molecule junction conductance. This talk will focus on the relation between molecular conductance and molecule conformation for the simple case of a biphenyl, two benzene rings linked together by a single C-C bond. Our results from a series of seven biphenyl derivatives show that the molecular junction conductance depends on the twist angle. Specifically, we find that the planar molecule has the highest conductance, and the conductance for the series decreases with increasing twist angle, consistent with a cosine squared relation predicted theoretically. 1. L. Venkataraman, J.E. Klare, I.W. Tam, C. Nuckolls, M.S. Hybertsen and M. Steigerwald, Nano Letters, vol. 5, pp. 458-462, 2006. 2. L. Venkataraman, J.E. Klare, C. Nuckolls, M.S. Hybertsen and M. Steigerwald, Nature, vol. 442, pp. 904-907, 2006.

3 NSF Nanoscale Science and Engineering Center at Columbia University and New York State Office of Science (NYSTAR)
11:51 AM B44.00002 DFT-based transport calculations for single molecules: Can Coulomb blockade effects be reproduced by local functionals?1, MAX KOENTOPP, Rutgers University, Dept of Chemistry, KIERON BURKE, UC Irvine, Dept of Chemistry — In principle, time-dependent current density functional theory (TDCDFT) allows for exact calculations of the electronic transport properties of single molecules. In practice, one is forced to make approximations for the exchange-correlation functional employed, and the computationally less costly ground-state DFT in a local approximation (GGA) is used. This introduces errors that can lead to an overestimation of the calculated current by one to two orders of magnitude. The use of local approximations to the exchange-correlation functional also leads to the inability to reproduce Coulomb blockade effects. We will discuss the origin and scope of these errors. Then, model calculations for molecules where Coulomb blockade effects have been observed experimentally will be presented, and the mechanism for the failure to reproduce Coulomb blockade effects will be explained.

1This work is supported by DOE (DE-AC02-05CH11231), NSF (DMR-0551195, DMR-04-39768, CHE-0117752), NYSTAR and NERSC.

12:03PM B44.00003 First-principles Studies of Single-molecule Conductance in Amine Linked Junctions1, SU YING QUEK, The Molecular Foundry, Lawrence Berkeley National Lab, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Lab and Columbia University, LATHA VENKATARAMAN, Physics Department, Columbia University, MICHAEL STEIGERWALD, COLIN NUCKOLLS, Chemistry Department, Columbia University, STEVEN G. LOUIE, Physics Department, University of California, Berkeley and Lawrence Berkeley National Lab. J.B. NEATON, The Molecular Foundry, Lawrence Berkeley National Lab. — Recently, it was discovered that the conductance of single molecule junctions with amine linkages to Au electrodes can be reliably and reproducibly measured. We compute and examine the conductance of prototypical single molecule junctions formed with amine-Au links using a first-principles scattering state method based on density functional theory. In particular, we elucidate the nature of the scattering states that give rise to the computed conductance, and relate the transmission spectra of each junction to intrinsic molecular and amine link properties. We explore the sensitivity of our results to specific contact geometries. The results are discussed relative to the measured distribution of conductance for each molecule.

1This work is supported by DOE (DE-AC02-05CH11231), NSF (DMR-0551195, DMR-04-39768, CHE-0117752), NYSTAR and NERSC.

12:15PM B44.00004 Electronic transport through alkane chains: the case of end group functionalization, G. KIM, W. LU, S. WANG, M. BUONGIORNO NARDELLI, J. BERNHOLC, Dept. of Physics, NC State Univ. — Using first-principles calculations, we have investigated the mechanism of metal/molecule coupling and its influence on the electronic transport properties in the prototypical case of long hydrocarbon (alkane) chains sandwiched between gold contacts. In our study, 1-Pentanethiol [CH$_3$(CH$_2$)$_4$SH] and 1-Pentyamine [CH$_3$(CH$_2$)$_4$NH$_2$] octanediame [CH$_3$(CH$_2$)$_8$(NH)$_2$] and octanethiol [CH$_3$(CH$_2$)$_8$(SH)$_2$] are anchored to ideally terminated Au (111) surfaces in order to investigate the effects of the functionalization of the end groups on the conduction properties. The results indeed show that the end group functionalization plays a crucial role in controlling the electronic transport through the molecule: the effective contact resistance of the amine/Au system is much smaller than that of the thiol/Au one, giving rise to a large difference in the I-V characteristics. Our results are in good agreement with recent experimental measurements of the tunneling current through these functional groups [1].

1C. Chu and G. Parsons, to be published (2006)

12:27PM B44.00005 ABSTRACT WITHDRAWN —

12:39PM B44.00006 Transport in Molecular Junctions with Different Metallic Contacts, JOHN LAWSON, CHARLES BAUSCHLICHER, NASA Ames Research Center — Ab initio calculations of phenyl dithiol connected to Au, Ag, Pd, and Pt electrodes are performed using non-equilibrium Green’s functions and density functional theory. For each metal, the properties of the molecular junction are considered both in equilibrium and under bias. In particular, we consider in detail charge transfer, changes in the electrostatic potential, and their subsequent effects on the IV curves through the junctions. Gold is typically used in molecular junctions because it forms strong chemical bonds with sulfur. We find however that Pt and Pd make better electrical contacts than Au. The zero-bias conductance is found to be greatest for Pt, followed by Pd, Au, and then Ag. (Physical Review B, 74, (2006), p 125401)

12:51PM B44.00007 Effects of -NO$_2$ substitution on charge addition and reorganization energies in phenylene ethynylene oligomers, STEVEN ROBEY, NIST-Gaithersburg, N. E. GRUHN, University of Arizona, J. CIZEK, Rice University, J. M. TOUR, Roise University — Reports of non-linear transport in molecular-scale junctions have stimulated suggestions for computing and switching applications based on molecular electronics. One of the most widely referenced results is reported negative differential resistance (NDR) behavior in -NO$_2$ substituted oligo-phenylene ethynlenes (OPE). Theoretical work has invoked the importance of charge addition effects on conformation and electronic structure and polaronic effects to provide potential explanations for this behavior. We have investigated charge addition effects for pristine versus -NO$_2$ substituted OPE self-assembled monolayers using photoelectron spectroscopy in combination with “doping” with K. Results are consistent with differences arising from filling of levels associated with the -NO$_2$ group. We have investigated polaronic effects using photoelectron spectroscopy and optical absorption to guide calculations of reorganization energies for pristine versus -NO$_2$ substituted OPE’s. We find theoretical evidence for increased reorganization energy with -NO$_2$ substitution for anionic species by about 33 percent, with experimental values of the reorganization energy ranging from about 0.2 eV to 0.4 eV and theoretical values about 0.2 eV.

1This work is supported by the DOE, the NSF and by NYSTAR.
1:15PM B44.00009 Electronic transport through single molecules: effects of strain and contacts
HELIO CHACHAM, RONALDO BATISTA, MARIO MAZZONI, Departamento de Física, ICEX, Universidade Federal de Minas Gerais, Brazil, IGNACIO GARZON, Instituto de Fisica, Universidad Nacional Autonoma, MARCELA BELTRAN, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, PABLO ORDEJON, Institut de Ciencia de Materiales de Barcelona, EMILIO ARTACHO, Department of Earth Sciences, University of Cambridge — We will present theoretical investigations on single-molecule electron transport. We will focus on the following systems: a) Connected Au nanoparticles: we performed a first-principles study [1] of the electronic properties of lattices of Au nanoparticles functionalized by the conjugated molecules BDMT and BDC. Distinctive features of the electronic matrix elements for the two functionalized Au nanoparticles as a function of strain and the atomic contacts. b) Current rectification with symmetric molecules: In an interesting experiment, Reichet et al. [2] measured the current through symmetric organic molecules and obtained asymmetric IV curves when the Au contacts are pulled apart. We show, by means of first-principles calculations, that this effect can originate from the formation of small Au chains between the molecule and the Au surfaces in an asymmetric way. [1] R. J. C. Batista et al, Phys. Rev. Lett. 96, 116802 (2006). [2] J. Reichet et al., Phys. Rev. Lett. 88, 176804 (2002).

1:27PM B44.00010 Controlled Fabrication and High-Resolution Imaging of Molecular-Scale Three-Terminal Devices
DOUGLAS R. STRACHAN, DANVERS E. JOHNSTON, BETH S. GUITON, T.-H. PARK, M.J. THERIEN, PETER K. DAVIES, DAWN A. BONNELL, A.T. CHARLIE JOHNSON, University of Pennsylvania — One of the biggest challenges to developing molecular-scale three terminal devices is to precisely fabricate contacts to the molecular nanowires. Using the transmission electron microscope (TEM) in order to monitor their formation with high-resolution imaging in real time. The technique relies on computer-controlled electron imaging to produce the nanogap at room temperature. This TEM imaging allows us to monitor the dynamics of the device evolution, where the gaps remain ordered and clear of residue during the process. This work was supported by the National Science Foundation (NIRT Grant No. 0304531 and MRSEC award DMR05-20020).

1:39PM B44.00011 Movies of the Formation of Break Junctions
THTI TAYCHATANAPAT, K. I. BOLOTIN, F. KUDEMETH, D. C. RALPH, LASSP, Cornell University, Ithaca, NY 14853 — Breaking metal wires by electromigration is a useful technique for making contacts for single-molecule devices. However, some research groups have found that a high percentage of gaps formed during electromigration (10-30%) can contain metal nanoparticles which produce artifacts in the device's electrical characteristics that might be mistaken for molecular signals. Other groups, using slightly different electromigration protocols, observe these artifacts at much lower rates. Here we investigate this issue by examining the electromigration process in real-time using a scanning electron microscope. We provide direct confirmation for arguments that a critical parameter in controlling whether nanoparticles are formed within the device. By observing devices to which metal nanoparticles have been attached using linker molecules, we are also able to estimate the effective temperature experienced by molecular adsortates during electromigration.

1:51PM B44.00012 Formation of a Metallic Contact: Jump to Contact Revisited
C. UNTIEDT, M.J. CATURULA, M.R. CALVO, J.J. PALACIOS, Departamento de Fisica Aplicada, Universidad de Alicante, E-03690 Alicante, Spain, R.C. SEGERS, J.M. VAN RUITENBEEK, Kamerlingh Onnes Laboratorium, Leiden University, PO box 9504, NL-2300 RA Leiden The Netherlands — The process of adhesion between two metallic surfaces has been described so far as involving an instability leading to a jump from tunneling into contact[1,2]. In the last decade some experiments have shown that this is not always the case and sometimes the transition from tunneling to metallic contact goes smoothly[3-5]. We have observed that the configuration and material composition of the electrodes before contacts largely determines the presence or absence of a jump. Moreover, when jumps are found, preferential values of conductance have been identified. Through combination of experiments, molecular dynamics, and first-principles transport calculations we show how these conductance values are related with atomic contacts of either monomers, dimmers or double-bond contacts. These results provide basic understanding of fundamental interactions between surfaces at the nanoscale.[1] N. Agrait, et al. Phys. Rev. Lett. 77,541 (2001)[2]U. Landman et al. Science 248, 454 (1990)[3]G. Cross et al. Phys. Rev. Lett. 80, 4685 (1998) [4]A. Halbritter et al. Phys. Rev. B. 68, 035417 (2003) [5]L. Limot et al. Phys. Rev. Lett. 94, 126102 (2005).

2:03PM B44.00013 High Quality Nanogap Electrodes for Electronic Transport Measurements of Single Molecules
DANVERS E. JOHNSTON, DOUGLAS R. STRACHAN, BETH S. GUITON, PETER K. DAVIES, TAE HONG PARK, MICHAEL J. THERIEN, A. T. CHARLIE JOHNSON, University of Pennsylvania — Electromigrated metal electrodes and resulting devices have shown great promise in moving towards the realization of single molecule-based electronic devices holding the potential for a wide range of electronic applications. At present, a major concern is that the electronic behavior of such devices may be greatly influenced by residual nanoscale metal particles. We have developed a computer controlled electromigration (CCE) circuit for monitoring the formation of nanogaps at room temperature which allows us to characterize a bare nanogap before putting a molecule into the nanogap. 1 This is very different from other approaches used in the field where nanogaps are formed at low temperature with molecules already attached to the nanowire by using a slow ramp up in voltage. Among the bare nanogaps we produced using CCE, tunneling behavior is observed with no indication of Single Molecules

2:30PM D3.00001 Organic-based Magnets - New Materials for New Physics
JOEL S. MILLER, University of Utah — Organic-based materials exhibiting the technologically important property of bulk magnetism, including ferro-, ferrim-, and magnetism, have been prepared. These magnets are prepared via conventional organic chemistry methodologies, but unlike classical inorganic-based magnets do not require metallurgical processing, and are frequently soluble in conventional solvents (e.g., toluene, dichloromethane, acetonitrile, THF). They have saturation magnetizations that in some cases exceed twice that of iron metal on a mole basis as well as have coercive fields exceeding that of Co55m. Also magnets with critical temperatures exceeding room temperature have been prepared. In addition to an overview of the observed magnetic behaviors, numerous examples of magnets made from molecules will be discussed. These examples are well known magnetic properties observed for classical inorganic transition/rare earth metal based magnets, as well as some new, unexpected phenomena and combinations of properties not previously reported. The design of examples of these organic-based magnets will be discussed setting the stage for an overview of their unusual magnetic properties and new physics that will be discussed by Arthur J. Epstein.

3This continued support by the US DOE Office of Basic Energy Sciences (Grant Nos. DE-FG03-93ER45504, DE-FG02-01ER45931, DE-FG02-86ER45271), NSF (Grant No. 0553575a), and AFSOR (Grant No. F9500-06-1-0175) is acknowledged.
3:06PM D3.00002 Predictable and New Physics and Potential for Applications of Organic-based Magnets1. ARTUR J. EPSTEIN, Department of Physics and Department of Chemistry, The Ohio State University, Columbus, OH 43210-1117 — As discussed by Joel S. Miller in the previous talk, magnets utilizing organic groups with essential spin have been reported since the mid-1980's. Though initial organic-based magnets had magnetic ordering temperatures (Tc's) below 5K, organic-based magnets now have Tc's to above 400K. In addition to magnetic phenomena already known for conventional transition metal and rare earth magnets, organic-based magnets feature unique phenomena enabled by the shape and internal electronic structure of the organic molecules. Examples are illustrated with experimental results for magnets based on tetracyanethylene, [TCNE], which, as an anion has spin 1/2. For example, chains with spin containing molecules having relatively strong exchange within a chain and weak dipolar interaction with neighboring chains can have an unusual fractal ground state with unusual dynamics leading to 'coercive fields' approaching 3 tesla. In contrast to conventional magnets, the internal electronic structure of the molecules that make up a molecule-based magnet can be excited by light of the appropriate wavelength. This leads to changes of the spin state of the molecule and/or changes in the exchange interaction between molecules, opening up the concept of reversible light control of magnetism. Examples will be given from the M^+[TCNE]^- (z~2) (M = Mn, V) materials systems. Finally, we explore the new phenomena enabled by V^+^[TCNE]^- (z~2), a material with Tc up to 400K and for which films may be prepared using low temperature CVD. It is a semiconductor (room temperature resistivity and activation energy similar to silicon) and magnetization M(H,T) and coercive field are controlled by chemical composition. Magnetoresistance to 32 tesla supports that V[TCNE]^- is a "half-semiconductor" with fully spin polarized valence and conduction bands of interest for spintronics applications.

1 This work has had the continued support by the US DOE Office of Basic Energy Sciences (Grant Nos. DE-FG02-86ER45271 and DE-FG02-01ER45931, and AFOSR (Grant No. F9550-06-1-0175).

3:42PM D3.00003 A Brief History of the Harris Criterion A. BROOKS HARRIS, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — In this talk I will briefly review the "Harris criterion," which was given in a 1974 paper in J. Phys. C. This criterion indicates whether the critical exponents of a system at a phase transition are modified by the presence of locally random impurities. To frame the discussion and since the argument for the criterion is so simple, I will repeat its derivation here. Since some of those who quote the paper may not have actually read it in detail, I will discuss some of the applications given there to systems with randomness which have longer-range correlations and I will emphasize those aspects which are perhaps less well-known. Also, with the benefit of hindsight, I will slightly reinterpret some of the conclusions of the 1974 paper. To further put this work in context, I will discuss how the renormalization group indicated that this argument indeed captured the essential role of local randomness. Later work on longer range models fits in nicely with the criterion. Finally, I will briefly mention experimental studies of this criterion. Perhaps the appropriate general conclusion from all of this is that a sound qualitative argument can have an honored place along side technically exact solutions.

4:18PM D3.00004 Opportunities in Nanomagnetism1, SAMUEL D. BADER, Argonne National Laboratory — This talk addresses the challenges and scientific problems in the emerging area of nanomagnetism. [1] Included are fabrication strategies, and experiments that explore new spin-related behavior in metallic systems, as well as efforts to understand the observed phenomena. As a subfield of nanoscience, nanomagnetism shares many of the same basic organizing principles, such as geometric confinement, physical proximity, and chemical self-organization. These principles are illustrated by means of examples drawn from the quests for ultra-strong permanent magnets, ultra-high-density magnetic recording media, and nanobiomagnetic sensing strategies. As a final example showing the synergetic relationship to other fields of science, the manipulation of viruses to fabricate magnetic nanoparticles is presented. [1] S. D. Bader, Rev. Mod. Phys. 78, 1 (2006).

Monday, March 5, 2007 2:30PM - 5:30PM — Session D8 DMP: Superconductivity: STM of Cuprates

2:30PM D8.00001 Tunneling Spectroscopy on c-axis Y1−xCaBaxCu3O7−δ Thin Films: Evidence for Multiband Superconductivity1, J.H. NGAI, University of Toronto, W.A. ATKINSON, Trent University, J.Y.T. WEI, University of Toronto — We report scanning tunneling spectroscopy measurements on {001} oriented Y1−xCaBaxCu3O7−δ thin films at x = 0, 0.05, 0.15 and 0.20 Ca-doping at 4.2K. The tunneling spectra exhibit main-gap, sub-gap and satellite features which we analyze using a generic multiband tunneling model that accounts for the separate contributions of the plane and chain bands to the tunneling superconductance. Our analysis indicates that the sub-gap features could arise from the chain band density of states, while the satellite features could come from the plane band for a d2−y2−s+ pairing symmetry. The doping dependent evolution indicates that all three spectral features are set by a single parameter, which monotonically decreases with Ca-doping, suggesting that superconductivity in Y1−xCaBaxCu3O7−δ involves multiple bands.

1 This work supported by NSERC, CIAR

2:42PM D8.00002 Direct evidence for predominantly phonon-mediated pairing in high-temperature superconductors, GUO-MENG ZHAO, Department of Physics and Astronomy, CSULA — The spectra of the second derivative of tunneling current d2I/dV2 in the high-temperature superconductors YBa2Cu3O7−delta and Bi2Sr2CuO6+δ show clear dip and peak features due to strong coupling to the bosonic modes mediating electron pairing. The energies of all the peaks in the d2I/dV2-like spectra match precisely with the energies of the peaks in the phonon density of states obtained by inelastic neutron scattering. The results clearly demonstrate that the bosonic modes mediating the electron pairing are phonons and that high-temperature superconductivity arises primarily from strong coupling to multiple phonon modes.

2:54PM D8.00003 Inelastic tunneling spectroscopic imaging study of electron-lattice interactions in Bi2Sr2CaCu2O8+x, KAZUHIRO FUJITA, U. of Tokyo, J. LEE, Cornell U., K. MCELROY, U. of Colorado, J. SLEZAK, M. WANG, Cornell U., Y. AIURA, H. BANDO, AIST, Tsukuba, S. UCHIDA, U. of Tokyo, J. C. DAVIS, Cornell U., J. C. DAVIS, Cornell U. — We investigated impact of oxygen isotope effect on d0 of Bi2Sr2CaCu2O8+x films at 4.2K. The tunneling spectra exhibit main-gap, sub-gap and satellite features which we analyze using a generic multiband tunneling model that accounts for the separate contributions of the plane and chain bands to the tunneling superconductance. Our analysis indicates that the sub-gap features could arise from the chain band density of states, while the satellite features could come from the plane band for a d2−y2−s+ pairing symmetry. The doping dependent evolution indicates that all three spectral features are set by a single parameter, which monotonically decreases with Ca-doping, suggesting that superconductivity in Y1−xCaBaxCu3O7−δ involves multiple bands.

1 This work supported by the U.S. Department of Energy under contract #DE-AC02-06CH11357.

4:18PM D3.00004 Opportunities in Nanomagnetism1, SAMUEL D. BADER, Argonne National Laboratory — This talk addresses the challenges and scientific problems in the emerging area of nanomagnetism. [1] Included are fabrication strategies, and experiments that explore new spin-related behavior in metallic systems, as well as efforts to understand the observed phenomena. As a subfield of nanoscience, nanomagnetism shares many of the same basic organizing principles, such as geometric confinement, physical proximity, and chemical self-organization. These principles are illustrated by means of examples drawn from the quests for ultra-strong permanent magnets, ultra-high-density magnetic recording media, and nanobiomagnetic sensing strategies. As a final example showing the synergetic relationship to other fields of science, the manipulation of viruses to fabricate magnetic nanoparticles is presented. [1] S. D. Bader, Rev. Mod. Phys. 78, 1 (2006).

Monday, March 5, 2007 2:30PM - 5:30PM — Session D8 DMP: Superconductivity: STM of Cuprates

2:30PM D8.00001 Tunneling Spectroscopy on c-axis Y1−xCaBaxCu3O7−δ Thin Films: Evidence for Multiband Superconductivity1, J.H. NGAI, University of Toronto, W.A. ATKINSON, Trent University, J.Y.T. WEI, University of Toronto — We report scanning tunneling spectroscopy measurements on {001} oriented Y1−xCaBaxCu3O7−δ thin films at x = 0, 0.05, 0.15 and 0.20 Ca-doping at 4.2K. The tunneling spectra exhibit main-gap, sub-gap and satellite features which we analyze using a generic multiband tunneling model that accounts for the separate contributions of the plane and chain bands to the tunneling superconductance. Our analysis indicates that the sub-gap features could arise from the chain band density of states, while the satellite features could come from the plane band for a d2−y2−s+ pairing symmetry. The doping dependent evolution indicates that all three spectral features are set by a single parameter, which monotonically decreases with Ca-doping, suggesting that superconductivity in Y1−xCaBaxCu3O7−δ involves multiple bands.

1 This work supported by NSERC, CIAR

2:42PM D8.00002 Direct evidence for predominantly phonon-mediated pairing in high-temperature superconductors, GUO-MENG ZHAO, Department of Physics and Astronomy, CSULA — The spectra of the second derivative of tunneling current d2I/dV2 in the high-temperature superconductors YBa2Cu3O7−delta and Bi2Sr2CaCuO6+δ show clear dip and peak features due to strong coupling to the bosonic modes mediating electron pairing. The energies of all the peaks in the d2I/dV2-like spectra match precisely with the energies of the peaks in the phonon density of states obtained by inelastic neutron scattering. The results clearly demonstrate that the bosonic modes mediating the electron pairing are phonons and that high-temperature superconductivity arises primarily from strong coupling to multiple phonon modes.

2:54PM D8.00003 Inelastic tunneling spectroscopic imaging study of electron-lattice interactions in Bi2Sr2CaCu2O8+x, KAZUHIRO FUJITA, U. of Tokyo, J. LEE, Cornell U., K. MCELROY, U. of Colorado, J. SLEZAK, M. WANG, Cornell U., Y. AIURA, H. BANDO, AIST, Tsukuba, S. UCHIDA, U. of Tokyo, J. C. DAVIS, Cornell U., J. C. DAVIS, Cornell U. — We investigated impact of oxygen isotope effect on d0 of Bi2Sr2CaCu2O8+x films at 4.2K. The tunneling spectra exhibit main-gap, sub-gap and satellite features which we analyze using a generic multiband tunneling model that accounts for the separate contributions of the plane and chain bands to the tunneling superconductance. Our analysis indicates that the sub-gap features could arise from the chain band density of states, while the satellite features could come from the plane band for a d2−y2−s+ pairing symmetry. The doping dependent evolution indicates that all three spectral features are set by a single parameter, which monotonically decreases with Ca-doping, suggesting that superconductivity in Y1−xCaBaxCu3O7−δ involves multiple bands.

1 This work supported by the U.S. Department of Energy under contract #DE-AC02-06CH11357.
3:06PM D8.00004 Atomic Scale Investigation of the Effects of Pb doping in Bi$_2$Sr$_2$CuO$_{6+\delta}$  
W. D. WISE, KAMALESH CHATTERJEE, M. C. BOYER, MING YI, MIT, TAKESHI KONDO, Ames Laboratory, E. W. HUDDSON, MIT — In the study of the Bi-based high temperature superconducting cuprates, an incommensurate structural “supermodulation” that runs throughout the crystal can often lead to experimental complications, especially for scattering studies. In order to eliminate this problem, a fraction of the Bi atoms are occasionally substituted by Pb, leading to a suppression of the supermodulation. As even a relatively large substitution has only a modest effect on transition temperature, it is widely believed that this substitution has little or no direct effect on superconducting properties. We will present the results of temperature dependent scanning tunneling microscopy studies of Pb doped Bi$_2$Sr$_2$CuO$_{6+\delta}$ (Bi-2211) which demonstrate local spectroscopic variations associated with Pb doping. Although the exact cause of these variations is still unknown, we hypothesize that a modulated strain field due to the presence of Pb may play a role.

3:18PM D8.00005 Spectroscopic imaging STM study of Bi$_2$Sr$_2$La$_x$CuO$_{6+\delta}$  
JINHWAN LEE, K. FUJITA, LASSP, Cornell University, K. MCELROY, University of Colorado, Boulder, JINHO LEE, LASSP, Cornell University, J.W. ALLDREDGE, M. WANG, Cornell University, S. ILLANI, LASSP, Cornell University, H. EISAKI, Advanced Indian Science and Technology, S. UCHIDA, University of Tokyo, J.C. DAVIS, LASSP, Cornell University  — We will present the spectroscopic imaging STM data of near optimally doped, Ln-substituted Bi2211. The Ln (Lanthanide) atoms substituting the Sr atoms are known to cause out-of-CuO$_2$-plane lattice disorder and large variation of Tc (Tc(La)\sim34K, Tc(Gd)\sim3K). We will demonstrate how the coherence peaks, the gap maps, the quasi-particle interference, and the checkerboard electronic structures are affected by lattice disorder and varied Tc in these materials. We will also show, for Gd-Bi2211, how the above atomic scale spectroscopic features change at temperatures below and above Tc.

3:30PM D8.00006 $d^2I/dV^2$-STS measurements of isotope effect on the electron-lattice interaction(ELI) energy and the gap energy in Bi-2212  
JINHO LEE, Cornell University, K. FUJITA, University of Tokyo, Japan, M. WANG, Cornell University, K. MCELROY, University of Colorado, J. SLEZAK, Cornell University, J.-X. ZHU, A. V. BALATSKY, Los Alamos National Lab, H. EISAKI, JSPS, Japan, T. ICHIHASHI, University of Tokyo, Japan, J.C. DAVIS, LASSP, Cornell University  — We measured gap energy and the electron-lattice interaction(ELI) energy on the O$^{16}$ and O$^{18}$ substituted Bi-2212 single crystals using $d^2I/dV^2$-STS(Scanning Tunneling Spectroscopy). Bi-2212 crystals were from the same batch, and nearly optimally doped after O$^{16}$ and O$^{18}$ annealing under the same conditions. Tc's were around 88K in both crystals. While the ELI energy was shifted to ~ 4mV lower energy in O$^{18}$ substituted Bi-2212, we found the gap energy of ~ 38mV in both crystals virtually didn’t change. We also extracted gap energies from the quasi-particle(D) dispersions using QP interferences, and will determine weather this gap energy is altered by isotope substitution. The possible identity of the lattice mode will be addressed in the context of recent results from IR spectroscopy and ARPES.

3:42PM D8.00007 Local pairing and the origin of pseudogaps in Bi$_2$Sr$_2$Ca$_2$Cu$_{4+\delta}$O$_{8+\delta}$ probed with high-resolution STM measurements  
KENJIRO K. GOMES, ABHAY PASUPATHY, AAKASH PUSH, Princeton Nanoscale Microscopy Laboratory, Department of Physics, Princeton University, SHIMPEI ONO, YOICHI ANDO, CRIEPI, Japan, ALI YAZDANI, Princeton Nanoscale Microscopy Laboratory, Department of Physics, Princeton University  — The evolution of the local electronic density of states in Bi$_2$Sr$_2$Ca$_2$Cu$_{4+\delta}$O$_{8+\delta}$ has been measured as function of doping ($\delta$=0.12-0.22) and temperature (20-180K) using state-of-art variable temperature scanning tunneling microscopy (STM). These measurements allow us to first characterize of spatially varying energy gap in both the superconducting and non-superconducting states with temperature. From these observations, we are able to demonstrate that pseudogaps observed at optimal doping at temperatures as high as 50K above Tc due to pairing correlations. We have been able to extract a remarkably universal relation that describes the strength of local pairing to a local pairing temperature, for samples which are weakly underdoped to highly overdoped. With decreasing doping, we show that the evolution of the local electronic states with temperature cannot be captured with a single pairing energy scale, signaling the presence of another phenomenon, which is unrelated or perhaps competing with superconductivity.

3:54PM D8.00008 Spatially Inhomogeneous Collapse of Superconducting Gaps on the Nanoscale: Connection to Macroscopic Measurements on Bi$_2$Sr$_2$Ca$_2$Cu$_{4+\delta}$O$_{8+\delta}$  
ALI YAZDANI, ABHAY PASUPATHY, KENJIRO K. GOMES, AAKASH PUSH, Princeton University, SHIMPEI ONO, YOICHI ANDO, CRIEPI, Japan  — Using spatially resolved STM spectroscopy, we have mapped the superconducting correlations in Bi$_2$Sr$_2$Ca$_2$Cu$_{4+\delta}$O$_{8+\delta}$ to show that these correlations collapse in a spatially inhomogeneous manner with increasing temperature. These experiments provide valuable insight for understanding the results of spatially averaged measurements such as angle-resolved photoemission, vortex Nernst and field-induced diamagnetism on the same material system. The connection between nanoscale measurements and bulk parameters such as Tc angle-resolved photoemission, vortex Nernst and field-induced diamagnetism on the same material system. The connection between nanoscale measurements and bulk parameters such as Tc angle-resolved photoemission, vortex Nernst and field-induced diamagnetism on the same material system.

4:06PM D8.00009 Atomic-Position Tracking and Spectroscopy of Bi$_2$Sr$_2$Ca$_2$Cu$_{4+\delta}$O$_{8+\delta}$ across Tc  
ABHAY PASUPATHY, KENJIRO K. GOMES, AAKASH PUSH, Princeton University, YUSUKE MIYANO, University of Tokyo, Japan, ALI YAZDANI, Princeton University  — The inhomogeneous nature of the pairing in the Bi$_2$Sr$_2$Ca$_2$Cu$_{4+\delta}$O$_{8+\delta}$ system makes the precise characterization of the changes in the density of states at the superconducting transition difficult to measure. Thermal drift in a typical STM prevents the tracking of a specific area while varying the temperature. We have used a specially designed STM, as well as a controlled electrical and acoustic environment, to track the position of a single atomic site on the surface as the temperature is varied. Using this technique, we have been able to measure, for the first time, how the onset of superconductivity changes the local tunneling spectra at a specific site. These measurements enable us to extract changes to the local density of states at Tc independent of the normal state background. We will describe this technique and our measurements on the Bi$_2$Sr$_2$Ca$_2$Cu$_{4+\delta}$O$_{8+\delta}$ system for different doping concentrations.

4:18PM D8.00010 Real Space Mapping of Electronic States in Bi$_2$Sr$_2$La$_x$CuO$_6$ as a function of Temperature  
AAKASH PUSH, ABHAY PASUPATHY, KENJIRO K. GOMES, Princeton Nanoscale Microscopy Laboratory, Department of Physics, Princeton University, NY US, SHIMPEI ONO, YOICHI ANDO, CRIEPI, Tokyo, Japan, ALI YAZDANI, Princeton Nanoscale Microscopy Laboratory, Department of Physics, Princeton University, NY US  — We will present the single layer Bi$_2$Sr$_2$La$_x$CuO$_6$ system using high resolution scanning tunneling microscopy and spectroscopy at various temperatures. From these measurements, we have determined the evolution of the local density of states from the superconducting to the non-superconducting state. In this talk, we will describe the evolution of the gap and other spectroscopic features as a function of doping ($\delta$=0.2 to 0.9) and temperature (20-100K). Real space maps of the electronic states that show strongly modulated patterns will also be presented. These experimental results are used to determine the connection between the superconducting gaps and the pseudo-gaps in this compound. Finally, we will discuss the similarities and differences between the measurements on the single-layer Bi$_2$Sr$_2$La$_x$CuO$_6$ and the double-layer Bi$_2$Sr$_2$Ca$_2$CuO$_{6+\delta}$.

Work supported by NSF-DMR, and through PCCM-MRSEC at Princeton.
4:30PM D8.00011 Superconducting Scanning Tunneling Microscope – Josephson effect and High-Tc superconducting cuprate. HIKARI KIMURA, ROBERT DYNES, University of California, Berkeley, SHIMPEI ONO, YOICHI ANDO, CRIEPI. We have developed and characterized superconducting scanning tunneling microscope (STM) tips that consist of Pb coated Pt/Ir wires. We have observed the thermally fluctuated Josephson effects between a conventional superconductor and this superconducting STM. STM-based Josephson junctions formed between the superconducting STM tip and superconducting samples can be a powerful tool to detect both superconducting quasiparticles and the phase of the superconducting condensate via the Josephson effect on a length scale of nanometers. This technique is especially powerful when we study spatially inhomogeneous electronic systems such as High-Tc superconducting cuprates. In this talk we present data of the STM Josephson junctions formed between S-STM tips and both Pb/Ag films and NbSe2 single crystals. The former experiments give us the effective noise temperature Tn and the impedance of the environment around the junction, Zjn. The latter is a precursor to the Pb/IHTc cuprate Josephson junctions. We have derived the Ic/RN product of NbSe2 junctions using Tn and Zjn obtained as described above. Preliminary results of Bi2Sr2CaCu2O8+x single crystals by S-STM tips are also discussed. This work is supported by DOE Grant No. FDDE-FG02-05ER46194.

4:42PM D8.00012 STM Spectroscopy of Electron Doped Pr1−xLaCe1−xCuO4−δ. FRANCIS NIESTEMSKI, SHANKAR KUNWAR, VIDYA MADHAVAN, Department of Physics, Boston College. We present high resolution scanning tunneling spectroscopy (STS) of electron doped Pr1−xLaCe1−xCuO4−δ. We focus on x=0.12 doping (Tc ~ 25K) at various temperatures at and above 2K. Our data reveal both small and large gap behavior in the same sample. The magnitude of the smallest measured gap is consistent with superconducting gaps observed by other probes. The larger gaps are of varying magnitudes ranging from 10meV to 100meV or greater. We will discuss our observations in light of experimental data on similar PLCCO samples from ARPES and neutron scattering.

4:54PM D8.00013 Atomic Resolution Scanning Tunneling Microscopy of Electron-Doped Pr1−xLaCe1−xCuO4−δ. SHANKAR KUNWAR, FRANCIS NIESTEMSKI, VIDYA MADHAVAN, Boston College. The study of electron-doped superconductors offers a new window into the still intractable problem of high temperature superconductivity. While hole-doped high Tc superconductors have been extensively studied with scanning tunneling microscopy (STM), there has been very little atomic resolution STM data on electron doped superconductors. We present STM images of in situ cleaved Pr1−xLaCe1−xCuO4−δ (PLCCO), obtained with a low temperature (5.6K), ultra high vacuum (UHV) STM. Due to the post annealing process required for superconductivity, superconducting PLCCO is expected to contain between 0.1% to 1% of the oxide impurity phases, (Pr, Ce)xO3. Our STM data on superconducting PLCCO reveal a few different atomic scale features, some of which have a periodicity consistent with the lattice constant expected for the impurity phases. Spectroscopy performed on these areas reveal gaps in the meV energy range. Possible origins of these and the other atomic scale structures will be discussed in this talk.

5:06PM D8.00014 Tunneling spectroscopy of e-doped cuprates. LEI SHAN, YAN HUANG, YONG-LEI WANG, National Laboratory for Superconductivity, IOP, CAS, SHI-LIANG LI, JUN ZHAO, PENG-CHENG DAI, University of Tennessee and Oak Ridge National Laboratory, TN, HAI-HU WEN, National Laboratory for Superconductivity, IOP, CAS, NATIONAL LABORATORY FOR SUPERCONDUCTIVITY, IOP, CAS TEAM, UNIVERSITY OF TENNESSEE AND OAK RIDGE NATIONAL LABORATORY, TN COLLABORATION. Point-contact tunneling spectra were measured on electron-doped high Tc cuprates (NCCO and PLCCO). By phenomenological analysis, we found that the superconducting gap (Δc) definitely decreases towards zero in an almost universal law with continuously increasing temperature or magnetic field. At the fields above Hc2, a clear “pseudogap” was opened indicated by the obvious spectral losing below a characteristic energy scale (Δpg) which is much larger than Δc. All the phenomena observed here seem to be crucial to distinguish the mechanism of HTSC and need to be extensively studied on more doping levels.

5:18PM D8.00015 Competing Orders: Origin of the Non-Universal Low-Energy Pseudogap Phenomena in Cuprate Superconductors1. CHING-TZU CHEN, A. D. BEYER, N.-C. YEH, California Institute of Technology. The contrasting low-energy pseudogap phenomena and quasiparticle spectral characteristics between the electron- and hole-type cuprates remain an open issue in cuprate superconductivity. Here we review the experimental manifestation of various non-universal properties and show that a phenomenological model of coexisting density-wave orders with superconductivity can consistently explain these disparate observations. By incorporating quantum phase fluctuations and adopting realistic bandstructures, numerical simulations of the quasiparticle tunneling spectra reproduce the empirical observations for both types of cuprates. Specifically, by tuning the ratio of the density waves to superconductivity, we can account for the absence of low-energy pseudogap in electron-type cuprates and the presence of pseudogap in hole-type cuprates. We therefore conclude that competing orders play an important role in the rich phenomenology of cuprate superconductivity.

Monday, March 5, 2007 2:30PM - 5:30PM – Session D9 DMP: Superconductivity: Charge Order and Inhomogeneity Colorado Convention Center Korbel 1D

2:30PM D9.00001 What does charge order have to do with the mechanism of high temperature superconductivity? STEVEN KIVELSON, Stanford University, EDUARDO FRADKIN, University of Illinois — Charge order clearly “competes” with superconductivity under many circumstances. It always tends to suppress the superfluid stiffness of the superconducting state by localizing electrons that might otherwise participate in the superconducting condensate. Thus, where the superconducting Tc is determined by phase fluctuations, charge order suppresses Tc. However, there is suggestive experimental and theoretical evidence that charge ordering of just the right sort can enhance pairing, and hence “assist” superconductivity. Some of this evidence will be presented.

2:42PM D9.00002 How optimal inhomogeneity produces high temperature superconductivity. EDUARDO FRADKIN, Department of Physics, University of Illinois at Urbana-Champaign, STEVEN KIVELSON, Department of Physics, Stanford University — The role of Coulomb frustrated phase separation in doped Mott insulators, and especially the consequences of the resulting local electronic structures on the “mechanism” of high temperature superconductivity will be discussed. The resulting perspective on superconductivity in the cuprates, and on the more general theoretical issue of what sorts of systems can support high temperature superconductivity is discussed as are some of the general, qualitative aspects of the experimental lore which should constrain any theory of the mechanism. Finally, it is show how they are accounted for within the context of the present theory. Reference: S. A. Kivelson and E. Fradkin, “How optimal inhomogeneity produces high temperature superconductivity,” cond-mat/0507459, to appear as a chapter in “Treatise of High Temperature Superconductivity” by J. Robert Schrieffer and J. Brooks, to be published (Springer, 2006)
2:54PM D9.00003 Thermodynamic properties of inhomogeneous superconductors near their transition temperature, SRINIVAS RAGHU, REZA JAMEI, STEVEN, KIVELSON, Stanford University — Recently, scanning tunneling spectroscopy (STS) experiments have revealed suggestive evidence of the existence of superconducting gap inhomogeneities at low temperatures in some families of cuprate materials. The consequences of such inhomogeneity near the superconducting transition, however, remain an important and unresolved issue. Here, we study the effect of intrinsic gap inhomogeneities on the mean-field electronic specific heat (and other thermodynamic properties) in the vicinity of the superconducting transition. We consider a spatially-varying pairing interaction in a d-wave BCS model, solve the mean-field equations self-consistently for the magnitude of the gap function, and determine the thermodynamic properties of the system. As T approaches Tc, the coherence length grows, causing the system to become effectively more homogenous due to self-averaging; we explore the extent to which various types of inhomogeneity remain important or get washed out near Tc.

3:06PM D9.00004 Global phase diagram of the checkerboard Hubbard model, HONG YAO, Stanford, WEI-FENG TSAI, UCLA, STEVEN KIVELSON, Stanford — Local electronic structure (self-organized inhomogeneity) may play an essential role for the “mechanism” of high-Tc superconductivity. Moreover, in the limit of large inhomogeneity, well-controlled theoretical solutions of strongly interacting models can be obtained. We have computed the phase diagram of the checkerboard Hubbard model in the limit of small inter-cluster electron hopping, t', for all doping (x=hole density per site) and for all interaction strengths, 0≤U/t≤4.5. For 0≤x≤1/2, the existence of an effective pair attraction results in one of two d-wave superconducting ground states – either with nodal or without nodal quasiparticles. For Uc < U < Uc=18.6t, the ground state is a Fermi liquid of spin 1/2 fermions with two possible orbital flavors. Interestingly, around x=1/4 the ground state is a spin-1/2 antiferromagnet which also possesses alternating orbital currents on every other plaquette that spontaneously break time reversal symmetry. For U>Uc, the ground state is a Fermi liquid of fermions with spin-3/2, with a spin-3/2 antiferromagnet is favored near x=1/4. By including next nearest neighbor hopping, t3, within clusters, we can study the physics of particle-hole asymmetry. Strikingly, we find that increasing t3 increases the range of U for which hole doping leads to a superconducting state, but suppresses the range of U for electron doping. (For t3 →∞, the roles of electrons and holes are interchanged.)

3:18PM D9.00005 Superconductivity in zigzag CuO chains, EREZ BERG, STEVE KIVELSON, Stanford University — Superconductivity was recently discovered in Pr2BaCuOy with a maximum Tc of about 12K [1]. This material’s structure is identical to that of the high Tc superconductor YBCO—347. However, the cuprate nature of the superconductivity in YBCO is known to be insulating. Therefore it is believed that the superconductivity originates in the array of quasi-1d CuO chains and NMR experiments appear to corroborate this belief. In this work we study a microscopic model for a CuO double-chain (zigzag chain) using a combination of bosonization and numerics (DMRG). We derive a schematic phase diagram for this model, which exhibits a narrow doping region where superconducting correlations are dominant and a broader range where CDW correlations are dominant. Unlike the situation in the two-leg Hubbard ladder, superconductivity does not arise from the formation of a spin gap. Rather, it is related to a subtle order driven by magnetic interactions. The implications for experiment are discussed.


3:30PM D9.00006 Stripes near a Quantum Critical Point,ERICA W. CARLSON, Department of Physics, Purdue University, DAOXIN YAO, DAVID K. CAMPBELL, Departments of Physics and Electrical and Computer Engineering, Boston University — Competing tendency in strongly correlated materials can cause spontaneous nanoscale structure, pattern formation, and even long-range spatial order. We explore the magnetic excitation spectrum in the stripe phase of high-Tc cuprates. Using a semiclassical spin wave treatment, we calculate the dynamical spin structure factor for weakly coupled stripes. We find a characteristic hourglass magnetic excitation spectrum with high-energy peaks rotated by 45 degrees compared to the incommensurate stripes. The ratio of peak intensity is strongly peaked on the inner branches of the spin wave cones when coupling across the stripes is weak, so that the entire spin wave cone is not likely to be resolvable experimentally. (Phys. Rev. Lett. 97, 017003 (2006), Phys. Rev. B 73, 224255 (2006))

3:42PM D9.00007 s-Wave Superconductivity Phase Diagram for the Two Dimensional Inhomogeneous Attractive Hubbard Model, KARAN ARYANPOUR, UC Davis-SUNY Buffalo, THEREZA C. PAIVA, Instituto de Fisica, Universidade Federal do Rio de Janeiro, Brazil, WARREN E. PICKETT, RICHARD T. SCALFETTAR, UC Davis — We study s-wave superconductivity in the two-dimensional square lattice attractive Hubbard Hamiltonian for various inhomogeneous patterns of interacting sites at different concentration values f. Using the Bogoliubov-de Gennes (BdG) mean field approximation, we find the phase diagram for inhomogeneous interaction patterns in which the on-site interaction U takes on two values, Uf = 0, Uc = 1 − f as a function of electron occupation per site n and study the evolution of the phase diagram as f varies. In certain regions of the phase diagram, inhomogeneity results in a larger zero temperature averaged pairing amplitude and also the superconducting phase transition temperature Tc, relative to a uniform system with U = Uc on all sites. These effects are observed for stripe, checkerboard, and even random patterns of the attractive centers, suggesting that the pattern of inhomogeneity is unimportant. The phase diagrams also include regions where superconductivity is obliterated due to the formation of various charge ordered phases. We show that for certain regular inhomogeneous patterns, increasing temperature works against the formation of these charge ordered phases and as a result, can enhance superconductivity.

3:54PM D9.00008 Competition between charge order and superconductivity in La2/3Ba1/3CuO4, JUNGHO KIM, KAGEDA, University of Toronto, G.D. GU, C.S. NELSON, Brookhaven National Laboratory, T. GOG, D. CASA, CMC-CAT, Advanced Photon Source, YOUNG-JUNE KIM, University of Toronto, UOT TEAM, BNL COLLABORATION, CMC-CAT, APS COLLABORATION — Understanding the role of stripe physics in cuprate superconductors is believed to be essential in elucidating the superconducting mechanism of the cuprates. Despite the fundamental importance of charge ordering in the cuprates, a comprehensive examination of the relationship between charge stripes and superconductivity is still lacking. We have carried out a detailed investigation of temperature and magnetic field dependence of charge order in La2/3Ba1/3CuO4 utilizing high-resolution x-ray scattering. We find that the correlation length of the charge order exhibits unusual temperature and magnetic field dependence. Specifically, at zero field the correlation length decreases as the sample is cooled below ~12K, while it increases as magnetic field is applied in the superconducting phase. These observations suggest that the size of the charge ordered region seems to be inversely correlated with superconductivity. This finding clearly shows that static charge order competes with the superconducting ground state, and supports the microscopic phase separation picture discussed by the recent μSR work.

4:06PM D9.00009 On the dimensionality of spin and charge modulations in 1/8 doped lanthanum cuprates , BORIS FIN, Physics Department, University of Tennessee — I compare the standard one-dimensional stripe interpretation of elastic scattering experiments in 1/8 doped lanthanum cuprates with two-dimensional interpretations. One of them is known as grid[1,2] and the other one is the lattice of magnetic vortices[3]. Both can induce a 4x4 charge modulation similar to the one detected by scanning tunneling spectroscopy. The case of magnetic vortices, however, is favored against grid by a recent spin polarized neutron scattering experiment.

4:18PM D9.00010 Fluctuating Cu-O-Cu Bond model of high temperature superconductivity in cuprates, D. M. NEWNS, C. C. TSUEI, IBM T. J. Watson Research Center — Twenty years of research have yet to produce a consensus on the origin of high temperature superconductivity (HTS). However, several generic characteristics of cuprate superconductors have emerged as the essential ingredients of and/or constraints on any viable microscopic model of HTS. Besides a transition Tc of order 100 K, they include a d-wave superconducting (SC) gap with Fermi liquid nodal excitations, a pseudogap with d-symmetry and the characteristic temperature scale T∗, an anomalous doping-dependent oxygen isotope shift, nanometer-scale gap inhomogeneity, etc. The isotope shift implies a key role for oxygen vibrations, but conventional BCS single-phonon coupling is essentially forbidden by symmetry and by the on-site Coulomb interaction U. Hence the present work invokes nonlinear coupling of planar oxygen vibrations to the Cu-0 hopping integral t. A dominant Fluctuating Bond field emerges involving oxygen vibrational square amplitudes - and associated Cu-Cu t∗′ in a pattern of quadrupolar symmetry around a given Cu site. Such fluctuations in Cu-Cu bonds mediate d-wave pairing, leading to a d-wave SC gap, and an explanation of the anomalous isotope shift. A quadrupolar CDW generates a d-wave pseudogap related to T∗. Other salient features of HTS are also explained by our model. This work is to appear in Nature Physics.

4:30PM D9.00011 Pair Binding in Small Hubbard Clusters, W.-F. TSAI, Dept. of Physics, UCLA, H. YAO, S. KIVELSON, Dept. of Physics, Stanford Univ, A. LAUCHLI, IRRMA, EPF Lausanne, Switzerland — One of the key issues in high-Tc superconductors is how (and whether) high temperature pairing can arise in an electronic system with only repulsive interactions. Here, we report the results of analytic and numerical exact diagonalization studies of small Hubbard clusters (up to 16 sites). Taking the N-electron ground-state as the ‘vacuum state’ of the cluster, we define the effective interaction between two added electrons to be Veff(N) = E(N+2)–E(N)–2E(N+1), where E(N) is the ground-state energy with N electrons on the cluster. Not surprisingly, for most clusters and most values of N, Veff(N) is repulsive (Veff(N) > 0), but there exist special clusters in which, for special N and in an appropriate range of U/t, there is an effective attraction, Veff(N) < 0. In the weak coupling limit (U/t<1), the results can be understood within perturbation theory, and the effective attraction, where it is occurs, is associated with the existence of an anomalous “resonantly entangled” groundstate. In the strong coupling limit, Veff(N) is always positive (or zero) due to Nagaoka physics. In some sense, the optimal cluster is the Hubbard-tetrahedron, for which Veff(N) is negative for all U/t. Finally, by studying the dependence of Veff(N) on the patterns of inhomogeneous couplings within a single cluster, we obtain some insight into the issue of whether there exists an optimal inhomogeneity for high-Tc superconductivity.

4:42PM D9.00012 Searching for orbital currents in the pseudo-gap state of Lax2−xSrxCuO4, G.J. MACDOUGALL, G.M. LUKE, A.A. ACZEL, J. RODRIGUEZ, McMaster University, J. Y. UEMURA, I. CARLO, T. ITO, Columbia University, P.L. RUSSO, TRIUMF, S. WAKIMOTO, University of Tokyo — Among the many outstanding riddles involving the cuprate materials is the microscopic nature of the so-called ‘pseudo-gap state’. Several theories have been put forth over the years, including pre-formed pairs, superconducting fluctuations and several branches of unconventional order. An example of the latter which has been getting particular attention of late is the idea that the pseudo-gap corresponds to an ordering of orbital currents. This renewed debate is mostly due to recent polarized neutron data on YBa2Cu3O7−δ, which claims to support a current ordered state which does not break translational invariance [PRL 96, 197001 (2006)]. These neutron results are not universally accepted, however, and clarifying experiments are necessary. In this spirit, we performed zero-field µSR on Lax2−xSrxCuO4 crystals with a wide range of Tc values, and searched for the spontaneous magnetic fields that would necessarily be associated with current order. We present the results of this search and discuss the implications our data for the interpretation of past and future experiments.

4:54PM D9.00013 The effect of inhomogeneous pairing amplitude on superfluid stiffness in a d-wave superconductor, MING CHENG, WU-PEI SU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204 — To explain the disparity between Tc and T∗ in optimally doped and underdoped cuprates, we propose that Tc is related to superconducting gap amplitude standard deviation (σ); while T∗ is related to average gap amplitude. We calculate the superfluid stiffness (μB) using BdG formalism for a d-wave superconductor. The calculations show that μB decreases as (σ) increases, suggesting lower Tc for more inhomogeneous gap distribution. The theoretic result is consistent with recent STM experiments which study the electronic inhomogeneities due to out-of-plane disorder.

5:06PM D9.00014 The Ground State of the Pseudogap in Cuprates, T. VALLA, Brookhaven National Laboratory, A. V. FEDOROV, Lawrence Berkeley National Laboratory, JINHO LEE, J. C. DAVIS, Cornell University, G. D. GU, Brookhaven National Laboratory — In conventional superconductors, the appearance of an energy gap in the electronic spectrum indicates pairing of electrons into Cooper pairs and a simultaneous transition into a macroscopic superconducting state. In contrast, in the underdoped high temperature superconductors, an energy gap is already present in the normal state. An understanding of this normal state gap or ‘pseudogap’ has proven elusive, because its ground state electronic structure was unknown. Here, we present studies of electronic structure in Lax2−xBaxCuO4, a unique system where the superconductivity is strongly suppressed and static spin and charge orders or ‘stripes’ develop near a doping level of x =1/8. Using angle-resolved photoemission and scanning tunneling microscopy, we detect an energy gap at the Fermi surface with magnitude consistent with d-wave symmetry and with linear density of states, vanishing only at four nodal points, even when superconductivity disappears at x =1/8. Thus, the non-superconducting, ‘striped’ state at x =1/8 is consistent with a phase incoherent d-wave superconductor whose Cooper pairs form spin/charge ordered structures instead of becoming superconducting.

1This work was supported by the DOE, Cornell University and ONR.

5:18PM D9.00015 The effects of local inhomogeneities on the phonon modulated DOS in Bi2212, STEVEN JOHNSTON, THOMAS DEVEREAUX, University of Waterloo — Recent scanning tunneling microscopy experiments on Bi2212 have revealed microscopic inhomogeneities in the local density of states and anomalous signatures of coupling to a bosonic mode. Gap referenced estimates for the mode energy are negatively correlated with the local gap size and the distribution of the mode estimates shows a clear isotope shift upon 18O substitution. Motivated by the clear isotope effect we examine electron-phonon coupling to the 55 meV apical oxygen mode in Bi2212 within the framework of Migdal-Eliashberg theory. The interplay of this interaction with local inhomogeneous broadening effects are also considered. The effects of the local dopant atoms on the electron-phonon interaction strength are examined using the Ewald summation technique.

Monday, March 5, 2007 2:30PM - 4:54PM
Session D10 DMP: Theory and Simulations of Systems with Disorder Colorado Convention Center Korbel 1E
2:30PM D10.00001 Percolation transition and dissipation in quantum Ising magnets

JOSE HOYOS, THOMAS VOJTA, University of Missouri-Rolla — We study the effects of dissipation on a randomly diluted transverse-field Ising magnet close to the percolation threshold. For weak transverse fields, a novel percolation quantum phase transition separates a superparamagnetic cluster phase from an inhomogeneously ordered ferromagnetic phase. The properties of this transition are dominated by large frozen and slowly fluctuating percolation clusters. This leads to a discontinuous magnetization-field curve and exotic hysteresis phenomena as well as highly singular behavior of magnetic susceptibility and specific heat. We compare our results to the smeared transition in generic dissipative random quantum Ising magnets. We also discuss the relation to metallic quantum magnets and other experimental realizations.

1Supported by the NSF under grant no. DMR-0339147

2:42PM D10.00007 Mott and Band Insulator Transitions in the Binary Alloy Hubbard Model

ANDREW BALDWIN, RICHARD SCALETTER, NORMAN PARIS, University of California, in Davis — We use determinant Quantum Monte Carlo simulations and exact diagonalization to explore insulating behavior in the Hubbard model with a bimodal distribution of randomly positioned local site energies. From the temperature dependence of the compressibility and conductivity, we show that gapped, incompressible Mott insulating phases exist away from half filling when the variance of the local site energies is sufficiently large. The compressible regions around this Mott phase are metallic only if the density of sites with the corresponding energy exceeds the percolation threshold, but are Anderson insulators otherwise.

3:30PM D10.00006 The geometrically-averaged density of states as a measure of localization

RACHEL WORTIS, YUN SONG, WILLIAM ATKINSON, Trent University — Motivated by current interest in disordered systems of interacting electrons, we examine the use of the geometrically-averaged density of states, \( \rho_g(\omega) \), as an order parameter for the Anderson transition. In infinite systems, when \( \rho_g(\omega) \) vanishes, while the density of states remains nonzero, the states at energy \( \omega \) are localized. In the context of noninteracting finite-size systems we show that a finite energy resolution, a common feature of many-body calculations, changes the scaling of \( \rho_g(\omega) \) such that the critical disorder is over-estimated. Furthermore we demonstrate that even in infinite systems a decline in \( \rho_g(\omega) \) with increasing disorder strength is not uniquely associated with localization.

1NSERC of Canada and Trent University

3:42PM D10.00004 Quantum Monte Carlo Study of a Magnetic-Field-Driven 2D Superconductor-Insulator Transition

KWANGMOO KIM, DAVID STROUD, The Ohio State University — Using quantum Monte Carlo calculations of the (2 + 1)-D XY model, we study the superconductor-insulator phase transition of a disordered 2D superconducting film vs. the applied magnetic field. The XY coupling is assumed to be \( -J \cos(\theta_i - \theta_j - A_{ij}) \), where \( A_{ij} \) has a standard deviation \( \Delta A_{ij} \). The critical coupling constant \( K_c = \sqrt{J/(2\Omega)} \). The universal conductivity \( \sigma^* \) is found to increase monotonically with \( \Delta A_{ij} \). Beyond a certain critical value of \( \Delta A_{ij} \), the superfluid density vanishes for all \( K' \)'s, but a renormalized coupling constant \( g \) remains finite, suggesting a transition into a Bose glass phase. At a larger value of \( \Delta A_{ij} \), the system becomes a Mott insulator. The critical values are found to be \( K_c = 0.490 \pm 0.001 \) and \( g^*/\sigma_Q = 0.324 \pm 0.003 \) when \( \Delta A_{ij} = 1/2 \); \( K_c = 0.532 \pm 0.001 \) and \( g^*/\sigma_Q = 0.494 \pm 0.011 \) when \( \Delta A_{ij} = 1/\sqrt{2} \); \( K_c = 0.585 \pm 0.004 \) when \( \Delta A_{ij} = 0.854 \); and \( K_c = 0.630 \pm 0.002 \) when \( \Delta A_{ij} = \infty \). The last value, which represents a Bose glass to Mott insulator transition, is obtained from \( g \), whereas the others represent a superconductor-to-insulator transition and are obtained from the superfluid density. We conclude that, for certain couplings, a disordered film may undergo a transition from superconductor to Bose glass to insulator with increasing field.

1Supported by NSF Grant DMR04-13395 and OSC.

4:2PM D10.00002 Nature of triplet excitations in the diluted 2D Heisenberg model

LING WANG, ANDERS SANDVIK, Boston University — We study the nature of ground state excitations of the 2D S=1/2 Heisenberg model on percolating clusters. We have previously argued that they involve weakly interacting localized moments, which are formed due to local sublattice imbalance [1]. We here discuss further confirmation of this picture for clusters with singlet ground states. First, we study a hard-core classical dimer-monomer model on percolating clusters. We find that the monomers are localized in small regions of local sublattice imbalance, and these regions coincide with regions of small local gaps (large local magnetic susceptibility), thus supporting the existence of localized magnetic moments due to sublattice imbalance. Second, we use quantum Monte Carlo simulations in the valence bond basis [2], with which we can study the spatial distribution of a triplet bond in the lowest-energy excited state. We find that the triplets are localized predominantly in a subset of the regions of localized monomers, supporting the notion that the lowest excitation is the singlet-triplet excitation of a small number of interacting effective moments. Supported by NSF grant DMR-0513930.


5:24PM D10.00003 Monte Carlo Study of Entanglement Scaling in Random S=1/2 Heisenberg Chains

HUAN TRAN, NICHOLAS BONESTEEL, Dept. of Physics and NHMFL, Florida State University — We present the results of a quantum Monte Carlo study of the S=1/2 Heisenberg chain with random antiferromagnetic nearest-neighbor coupling. Using the method of ground state projection in the singlet-bond basis, recently introduced by Sandvik [3] we are able to directly confirm the expected freezing of the ground state into a random singlet phase at long length scales, while at the same time exactly capturing the nonuniversal (i.e. detail dependent) short-range bond fluctuations. By computing the bond-length distribution in the random singlet phase we are then able to determine the mean entanglement entropy, \( S_N \), associated with a segment of \( N \gg 1 \) spins, both by self-averaging over segments for a particular realization of disorder, and by averaging over many distinct realizations of disorder. Our results confirm the \( S_N \approx \ln^2 N \) scaling found by Refael and Moore using real space RG [4] showing that the "effective central charge" of the critical random S=1/2 Heisenberg chain is \( c = 1/2 \). Work supported by US DOE.

of the oxygen octahedra surrounding the Mn cations. The resulting two-band model is then applied to study LaMnO$_3$ physically transparent tight binding model and considering both nearest and next nearest neighbor hoppings. In particular, we address effects due to rotations by the superlattice affect the orbital and magnetic orders. This work is supported by DMR-0213574.

electron-electron interactions within those bands. We will show how charge reconstruction, structural constraints and the symmetry breaking induced by the superlattice affect the orbital and magnetic orders. This work is supported by DMR-0213574.

4:06PM D10.00009 Local defect in a magnet with long-range interactions. THOMAS VOJTA, JOSE HOYOS, Dept. of Physics, University of Missouri-Rolla — We investigate a single defect coupling to the square of the order parameter in a nearly critical magnet with long-range spatial interactions of the form $r^-(d+s)$ focusing on magnetic droplets nucleated at the defect while the bulk system is in the paramagnetic phase. Because of the long-range interaction, the droplet develops a power-law tail which is energetically unfavorable. However, as long as $s > 0$, the tail contribution to the droplet free energy is subleading in the limit of large droplets; and the free energy becomes identical to the case of short-range interactions. We also study the droplet quantum dynamics with and without dissipation; and we discuss the consequences of our results for defects in itinerant quantum ferromagnets.

4:18PM D10.00010 “Exact” algorithm for random-bond Ising models in 2D. YEN LEE LOH, ERICA W. CARLSON, Purdue University — For nearly 80 years the Ising model and its variants have given valuable insight into phase transitions and critical phenomena in magnets, alloys, and many other systems. Random-bond Ising models (RBIMs) in particular are often used to study frustration and spin-glass behavior, and they are closely related to neural networks and information theory. We present an algorithm for solving two-dimensional Ising models with any configuration of bond strengths [1]. The algorithm is an extension of the bond-propagation algorithm originally developed for resistor networks [2]. It calculates the partition function and correlation functions at a single temperature for any planar Ising model of linear dimension $L$ in $O(L^3)$ time or less. The results are numerically exact (subject only to roundoff error). The method is especially efficient for dilute models near the percolation threshold, for which it executes in $O(L^2 \ln L)$ time. Moreover, it operates directly in the spin basis, without the need for mapping to fermion or dimer models, and it is massively parallelizable. It gives fresh insight on the peculiar “hidden integrability” of 2D Ising models and suggests new directions for tackling other problems.

4:30PM D10.00011 Quenched disorder and structure of short-range spin correlations. IGOR ZALIZNYAK, Brookhaven National Laboratory — In many important cases, magnetic order existing in a crystal does not possess long-range coherence, but has short-range nature. In particular, such is the situation in a variety of doped perovskite oxides, including cuprates, nickelates and cobaltates, which have recently been extensively studied in view of their fascinating electronic properties. In the absence of macroscopic spin coherence, the Fourrier-transform of spin-spin correlation in the crystal, which determines elastic magnetic scattering measured in experiment, does not contain delta- functions giving rise to magnetic Bragg peaks. Instead, it contains broad diffuse peaks which experimenters usually describe by phenomenological profiles, such as Lorentzian, Lorentzian-squared, etc., some of which are only appropriate in the near vicinity of the peak position (e.g. in the Orstein- Zernike approximation). Here we consider a simple model of quenched disorder introduced by a system of static magnetic disclinations/stacking faults of various symmetry and dimensionality. The corresponding spin correlation function has a form of the “lattice-Lorentzian,” where the Lorentzian’s power is determined by the dimensionality of the disorder.

4:42PM D10.00012 Simulation on depinning of a magnetic domain wall based on Heisenberg spin model. KATSUYOSHI MATSUSHITA, XIAO HU, National Institute for Materials Science — Motion of magnetic-field driven magnetic domain-wall subject to random pinning centers has attracted much attention. One of the characteristic phenomena in the system is the depinning transition at non-zero pinning force. It is expected that such motion can be described by an elastic deformable interface in a disordered medium. The depinning transition of a magnetic domain wall in an Ising spin system with random pinning fields has been studied which confirmed this expectation. In the present study, by using Monte Carlo and molecular dynamics simulations, we investigate motion of a domain wall in a Heisenberg spin system. In contrast to the Ising case, we observed discontinuous jump in domain-wall velocity upon depinning. Simulation results will be presented and the physics behind the difference will be discussed.

Monday, March 5, 2007 2:30PM - 5:30PM – Session D11 DMP: Focus Session: Correlated Electron Superlattices

2:30PM D11.00001 A tight-binding LDA+DMFT study of manganite superlattices. CLAUDE EDERER, CHUNGWEI LIN, ANDREW MILLIS, Columbia University — The combination of ab initio density functional theory with model “many-body” calculations provides a very promising way for a realistic theoretical treatment of surface and interface effects of strongly correlated electron materials. Here we show in detail how the electronic structure of LaMnO$_3$ calculated within the local density approximation (LDA) can be efficiently parametrized using a physically transparent tight binding model and considering both nearest and next nearest neighbor hoppings. In particular, we address effects due to rotations of the oxygen octahedra surrounding the Mn cations. The resulting two-band model is then applied to study LaMnO$_3$:SrMnO$_3$ superlattices using dynamical mean-field theory (DMFT) and the predicted ground state phases for superlattices with a small number of individual LaMnO$_3$ and SrMnO$_3$ layers are compared with the results obtained by density functional theory.

2:42PM D11.00002 A Realistic Model Calculation on Manganese Superlattice. CHUNGWEI LIN, CLAUDE EDERER, ANDREW MILLIS, Columbia University — We present a realistic model calculation for (0,0,1) LaMnO$_3$ (SrMnO$_3$)$_n$ superlattices. In this model, the superlattice is defined by the long-range Coulomb interaction generated by different ion charges of La (3+) and Sr (2+). The electronic degree of freedom contains two Manganese-Oxygen hybridized $e_g$ bands coupled to localized Mn $t_{2g}$ spins and to Jahn-Teller phonon modes, and the most general on-site electron-electron interactions within those $e_g$ bands. We will show how charge reconstruction, structural constraints and the symmetry breaking induced by the superlattice affect the orbital and magnetic orders. This work is supported by DMR-0213574.
Two-dimensional spin-polarized electron gas at the perovskite manganite interface: SrMnO$_3$/LaMnO$_3$ | BIRBARAB NANDA, Department of Physics, University of Missouri, Columbia (MO), SASHI SATPATHY, Department of Physics, University of Wisconsin, Madison (WI) — Electronic structure calculations for the perovskite manganite heterostructure (SrMnO$_3$)$_n$/(LaMnO$_3$)$_m$/(SrMnO$_3$)$_n$ reveal the presence of a novel spin-polarized electron gas at the interface, generated from the stripped-off La (Sr$^+$) electrons, which become confined in the electrostatic V-shaped potential well of the positively charged (LaO) sheet, occupying the Mn($e^-$) states near the interface. The presence of these electrons turns the interaction between the interfacial Mn atoms to be ferromagnetic via the Anderson-Hasegawa double exchange, overcoming the original antiferromagnetic superexchange present in the SrMnO$_3$ bulk. The FM Mn atoms at the interface in turn make the electron gas spin-polarized, as confirmed by the total energy calculations, and the type G AFM of the bulk is resumed a few layers into the bulk.

This work was supported in part by the U. S. Department of Energy under Grant No. DE-FG02-00ER45818.

First-principles study of LaAlO$_3$/SrTiO$_3$ thin films | KRISTOPHER ANDERSEN, C. STEPHEN HELLBERG, Naval Research Laboratory — Although the perovskite oxides LaAlO$_3$ (LAO) and SrTiO$_3$ (STO) are conventional band insulators, an electron gas can form at their interface. Several mechanisms have been proposed to produce the electron gas, including the electrostatic divergence within LAO that results from the growth of alternating charged (LaO)$^+$ and (AlO)$^-$ layers and an electronic reconstruction in which Ti$^{4+}$ and Ti$^{3+}$ is formed at the interface. Of practical interest, thin films of LAO on STO have been observed to have highly mobile carriers and a carrier density that is tunable via LAO thickness—in recent work, Thiel et al. observed an insulator-metal transition between 3–4 MLs. In this talk, first-principles electronic structure calculations are performed on LAO thin films grown on STO to investigate surface reconstructions and the penetration depth of the electron gas into the substrate. An insulator-metal transition is found in good agreement with experiment.

Theory of band alignment at the LaAlO$_3$/SrTiO$_3$ interface | JAEKWANG LEE, ALEX DEMKOV, The University of Texas — A polar discontinuity at the abrupt oxide/oxide interface is one of several problems that need to be addressed before we can realize the promise of multiforamic oxide structures. To avoid the so-called polar catastrophe the interface undergoes roughening which renders the structure useless, unless the system finds a mechanism for compensating the interface charges. Recent experiments of Hwang and co-workers (Nature 427, 423-426 (2004) and Nature 430, 657-661 (2004)) suggest that in the case of perovskite oxides two quite different compensatory mechanisms are at play at the heterojunction. For the n-type LaAlO$_3$/SrTiO$_3$ interface it is purely electronic involving mixed valence Ti ions, while for the p-type it is an actual ionic reconstruction involving oxygen vacancies. We present first-principles study of both interfaces within density functional theory. We consider the energetics and electronic structure of the interface, including the role of oxygen vacancies and band offsets. In addition we consider the interface stability with respect to interdiffusion of La and Sr across the interface.

Correlation driven charge order at LaAlO$_3$/SrTiO$_3$ and LaTiO$_3$/SrTiO$_3$ interfaces | ROSSITZA PENTCHEVA, Dept. of Earth and Environmental Sciences, Section Crystallography, University of Munich — Correlated behavior at complex oxide interfaces offers additional degrees of freedom to compensate charge imbalance not available e.g. in polar semiconductor heterostructures. This can result in electronic, charge and magnetic phases that do not exist in the bulk and offers new possibilities for device applications. For instance, the interfaces of LaTiO$_3$ and SrTiO$_3$ [1] as well as LaAlO$_3$ and SrTiO$_3$ [2] show metallic conductivity, although the respective bulk materials are Mott (LTO) and band insulating (STO, LAO). Here we present the results of material-specific correlated band theory (LDA+U) employing the FP-LAPW code in the WIEN2k implementation for a variety of (n,m) multilayers containing n LTO (or LAO) and m STO-layers. To explore the relaxation length towards bulk behavior n and m is varied between 1 and 9. We find that charge mismatch at the LTO/STO IF is accommodated by the formation of a charge and orbital-ordered (CO/OO) layer with a checkerboard arrangement of Ti$^{3+}$ and Ti$^{4+}$ and an antiferromagnetic coupling of the Ti$^{3+}$/Ti$^{4+}$ spins [3]. Lattice relaxations lead to the observed conducting behavior. An analogous diluted layer of Ti$^{3+}$/Ti$^{4+}$ spins is obtained for the n-type LAO/STO interface, although the corresponding bulk materials are nonmagnetic. For a structurally ideal p-type LAO/STO IF the measured insulating behavior can only be understood by a charge disproportionation on the oxygen sublattice and the formation of a CO/OO magnetic OPe hole. Alternatively, charge compensation by oxygen vacancies and the formation of a charge conjugate F-center is considered. [1] A. Ohtomo, and H. Y. Hwang, Nature 427, 423 (2004). [2] A. Ohtomo, D.A. Muller, J.L. Grazul, and H.Y. Hwang, Nature 419, 378 (2002). [3] R. Pentcheva and W.E. Pickett, cond-mat/0608212. [4] R. P. pentcheva and W.E. Pickett, Phys. Rev. B 74, 053112 (2006).

Origin of the charge carriers at LaAlO$_3$/SrTiO$_3$ hetero-interfaces: possibility of intrinsic doping | GERT JANSSEN, WALTER HARRISON, Stanford University, HIDEKI YAMAMOTO, NTT Basic Research Laboratories, WALTER HARRISON, Stanford University, GERALD LUCOVSKY, North Carolina State University, THEODORE GEBALLE, Stanford University, DAVE BLANK, University of Twente, and MALCOLM BEASLEY, Stanford University — We have made very thin films of LaAlO$_3$ on TiO$_2$ terminated SrTiO$_3$. In situ UPS, XAS, XES, transport measurements and annealing experiments results indicate that oxygen vacancies play an important role in the creation of the charge carriers and that these vacancies are induced by the slow laser deposition process. Our results explain for the first time the origin of the large sheet carrier densities and high mobility observed previously. Simple model calculations confirm the plausibility of having defects at the origin of charge carriers while still maintaining high a mobility. By means of annealing experiments in atomic oxygen we examine the question whether an intrinsically doped interface does indeed exist at lower carrier concentrations. Work supported by the DOE BES and EPRI.

Kondo effect and ferromagnetic ordering at the n-type SrTiO$_3$ - LaAlO$_3$ conducting interface | ALEXANDER BRINKMAN, MARK HUIJIBEN, MAARTEN VAN ZALK, JEROEN HUIJIBEN, WILFRED VAN DER WIEL, GUUS RUIJDERS, DAVE BLANK, HANS HILGENKAMP, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — The intriguing phenomenon of electrical conductivity at the interface between two insulators is one of the possible consequences of electronic reconstruction of materials. In analogy with interface conduction, the question arises whether or not it is possible to induce magnetism at the contact between two nonmagnetic materials. We show how a polar discontinuity at the n-type conducting interface between the nonmagnetic perovskites SrTiO$_3$ and LaAlO$_3$ can induce a local magnetic moment on the Ti site. The resulting interface magnetism manifests itself in the form of ferromagnetic ordering at 0.3 K and the scattering of conduction electrons on the magnetic local moment, which provides a large negative magnetoresistance of 30%. The scattering can be described in terms of the Kondo effect with a Kondo temperature of 50 K. Electronically reconstructed interfaces now provide another versatile class of solid state Kondo systems, next to dilute impurities in metals and artificial quantum dots.

Optical Conductivity of LaAlO$_3$/SrTiO$_3$ Superlattices | C.L.S. KANTNER, M. HUIJIBEN, J. SEIDEL, M. WARUSAWITHANA, D.G. SCHLOM, R. RAMESH, J. ORENSTEIN — Precise contactless measurements of the optical conductivity of LaAlO$_3$/SrTiO$_3$ (LAO/STO) superlattices can be made possible through the use of Si rather than STO substrates. To identify the interface contribution to the conductivity we compared the optical transmission of structures with different numbers of interfaces, while maintaining constant the total number of unit cells.
Interfaces between the band insulator SrTiO$_3$ and the antiferromagnetic charge-transfer insulator LaMnO$_3$ provide a particularly interesting platform to test such effects. Both perovskites are grown epitaxially by pulsed-laser deposition, and electron energy loss spectra (EELS) collected in a scanning transmission electron microscope (STEM) show interfacial valence changes on the Mn-sites, while Ti remains in a +4 state even in direct contact with the LaO layer of the LaMnO$_3$. This observation is fully consistent with computational results obtained for such structures using the self-interaction corrected (SIC) local spin density (LSD) method. In this presentation, we discuss the physical origin and consequences of these valence changes in single interfaces as well as LaMnO$_3$/SrTiO$_3$ superlattices. This research was sponsored by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory (ORNL), managed and operated by UT-Battelle, LLC, and ORNL’s Laboratory Directed Research and Development Program.

**4:42PM D11.00010 Properties of epitaxial LaMnO$_3$/SrTiO$_3$ interfaces.** HANS M. CHRISTEN, DAE HO KIM, HO NYUNG LEE, MARIA VARELA, LEON PETIT, THOMAS SCHULTHESS, Oak Ridge National Laboratory — Electronic effects at interfaces between dissimilar oxides are known to have fundamental consequences on their transport and magnetic properties. Interfaces between the band insulator SrTiO$_3$ and the antiferromagnetic charge-transfer insulator LaMnO$_3$ provide a particularly interesting platform to test such effects. Both perovskites are grown epitaxially by pulsed-laser deposition, and electron energy loss spectra (EELS) collected in a scanning transmission electron microscope (STEM) show interfacial valence changes on the Mn-sites, while Ti remains in a +4 state even in direct contact with the LaO layer of the LaMnO$_3$. This observation is fully consistent with computational results obtained for such structures using the self-interaction corrected (SIC) local spin density (LSD) method. In this presentation, we discuss the physical origin and consequences of these valence changes in single interfaces as well as LaMnO$_3$/SrTiO$_3$ superlattices. This research was sponsored by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory (ORNL), managed and operated by UT-Battelle, LLC, and ORNL’s Laboratory Directed Research and Development Program.

**5:06PM D11.00012 Band structure engineering of LaMnO$_3$/SrTiO$_3$ superlattices at the molecular level**

KUI-JUAN JIN, HUI-BIN LU, QING-LI ZHOU, GUO-ZHEN YANG, MENG HE, KUN ZHAO, Institute of Physics, Chinese Academy of Sciences — Different from the negative colossal magnetoresistance (CMR) of doped manganites, a positive CMR is discovered at low applied magnetic field and high temperature in the epitaxial $p-n$ heterostructure with Sr-doped LaMnO$_3$ and Nb-doped SrTiO$_3$ fabricated by laser molecular-beam epitaxy [1,2]. We have found that such unusual positive CMR is an interface effect which causes a charge redistribution in at the interface with different electron spin polarization at Fermi level from that in the corresponding bulk CMR materials. Self-consistent calculation was carried out the band structure around the interface of the heterostructure and confirms the unusual behavior. Other puzzling CMR features with bias voltage, temperature and even composition are well explained by the present scenario. 1. Kui-Juan Jin et al., Phys. Rev. B 71, 184428 (2005). 2. Qing-li Zhou, et al., Europhys. Lett. 71, 1-7 (2005)
The influence of quantum confinement on magnetism in quantum dots.\(^1\)
RAMIN ABOLFATH, IGOR ZUTIC, SUNY Buffalo, PAWEL HAWRYLAK, NRC Ottawa — Owing to its simplicity, the vast majority of theoretical studies of magnetically doped quantum dots imply parabolic shape of the quantum confinement. However, several methods of fabricating quantum dots are more appropriately described by other forms of quantum confinement that remain largely unexplored. To assess the influence of the choice of confining potential and its strength, we perform a systematic comparison of magnetic phases of quantum dots described by parabolic and Gaussian confinement. We focus on the magnetization, carrier spin polarization, and magnetic transition temperature. We clarify which of these quantities could be strongly modified by the choice of non-parabolic quantum confinement and predict related experimental implications \([1]\). Cond-mat/0612489.

\(^{1}\)Supported by US ONR and NSF ECCS.

Theory of phonon-induced spin relaxation in coupled lateral quantum dots\(^3\), JAROSLAV FABIAN\(^2\), Institute for Theoretical Physics, University Regensburg, 93040 Regensburg, Germany — Electron spins in lateral quantum dots at GaAs/GaAlAs interfaces relax in milliseconds. Spin relaxation here means transitions from the upper to the lower Zeman split orbital ground state, at an applied magnetic field. Both spin-orbit and electron-phonon couplings are needed for spin flips between spectrally distinct and opposite-spin states. We have carried out realistic numerical and analytical calculations of spin relaxation and spin dynamics in single and coupled lateral quantum dots \([1]\). Our results agree with existing experiments on single dots, while predict interesting effects for coupled dots. Most important, spin relaxation in coupled dots is dominated by spin hot spots—anticrossings of states of opposite spins—practical couplings (say, 0.1 meV). Spin hot spots reduce spin relaxation to nanoseconds! Fortunately, spin hot spots are strongly anisotropic and there can be (rather singular) configurations, we call them easy passages, in which spin relaxation slows down to milliseconds as in single dots. For a (001) plane, for example, an easy passage occurs if coupled dots are oriented along [110] and the in-plane magnetic field lies perpendicular, along [100]. This configuration should be used for spin-based quantum information processing. This easy passage also protects spin qubits from electrical field disturbances which occur in "on-chip" single electron spin resonance experiments, as will be demonstrated theoretically using density matrix formalism for electron spins in the presence of both dissipation and driving oscillating electric and magnetic field \([2]\).

\(^{2}\)P. Stano and J. Fabian, cond-mat/0611228.

Control of electron spin and orbital resonance in quantum dots through spin-orbit interactions\(^1\), PETER STANO, JAROSLAV FABIAN, University of Regensburg — Dynamics of a single electron in coupled lateral quantum dots in the presence of a static and oscillating electric and magnetic fields as well as phonon-induced relaxation and decoherence is investigated. Using symmetry arguments it is shown that spin and orbital resonance can be efficiently controlled by spin-orbit couplings. The so called easy passage configuration is shown to be particularly suitable for magnetic manipulation of spin qubits, ensuring long spin relaxation time and protecting the spin qubit from electrical field disturbances connected with on-chip manipulation.

\(^{3}\)Supported by US ONR.

Electron Spin Decoherence via Optical Phonons in Quantum Dots\(^1\), YURIY SEMENOV, KI WOOK KIM, North Carolina State University — Electron spin decoherence caused by elastic spin-phonon processes is investigated comprehensively in a zero-dimensional environment. Specifically, a theoretical treatment is developed for the processes associated with the anharmonic vibrations of optical phonons in the semiconductor quantum dots. The optical phonons possess relatively high energy that was reasons not involving them to the problem of quantum computing decoherence to present day. This is true if we associate spin decoherence with inelastic processes of spin relaxation that needs thermal activation of optical phonons. In the case of elastic processes the uncontrolled variation of spin phase can happen without presence of thermal phonons. Zero-point optical phonons possess relatively high energy that was reasons not involving them to the problem of quantum computing decoherence to present day. This is true if we associate spin decoherence with inelastic processes of spin relaxation that needs thermal activation of optical phonons. In the case of elastic processes the uncontrolled variation of spin phase can happen without presence of thermal phonons.

\(^{1}\)This work has been supported by the US ONR.

Towards Electrical Spin Injection into a Single InAs/GaAs Quantum Dot\(^2\), C. H. LI, G. KIOSEOGLOU, A. T. HANBICKI, O. M. J. VAN ‘T ERVE, B. T. JONKER, Naval Research Lab — We aim to isolate emission from a single InAs/GaAs self-assembled QD to elucidate the details of electrical spin injection from an Fe Schottky contact and consequent spin polarization in QDs. MBE growth methods have been developed to reduce the dot density to the order of 10\(^{10}\) cm\(^{-2}\), which in turn also increases the uniformity of the dots, allowing us to resolve their atomic-like s, p, d, f... quantum confined states. The aperture sizes of the surface-emitting LEDs are also reduced to the order of a hundred nanometers using ebeam lithography. As the density and aperture size decrease, the initially broad emission spectrum of the dot ensemble \([1]\) breaks into distinct narrow features attributed to single dot emission at low biases. With increasing bias, the number of peaks increases and their linewidth broadens, suggesting contributions from emission from an increasing number of dots and/or from various charge states of the dot. At even higher bias, the sets of peaks merge and approach broad emissions. Progress towards electrical spin injection into a single QD, and details of the electroluminescence spectra as a function of bias and magnetic field will be discussed at the meeting. \([1]\) C. H. Li et al. APL 86, 132503 (2005).

\(^{2}\)Supported by ONR and DARPA.

Quantum Point Contacts as Spin Injectors and Detectors for Studying Rasha Spin Precession in Semiconductor Quantum Wires, PHILIPPE DEBRAY, University of Cincinnati, Cincinnati, Ohio 45221, IVAN SHORUBALKO, HONGQI XU, Lund University, Sweden — We have studied polarized spin transport in a device consisting of three quantum point contacts (QPCs) in series made on InGaAs/InP quantum-well (QW) structures. The QPCs were created by independent pairs of side gates, each pair for one QPC. By adjusting the bias voltages of the side gates, the widths of the QPCs are independently tuned to have transport in the fundamental mode. An external magnetic field of a few T causes spin splitting of the lowest one-dimensional (1D) subbands. The widths of the end QPCs are adjusted to position the Fermi level in the spin-split energy gap, while that of the central QPC is kept wide enough to populate both spin-split bands. Measurement of the conduction of the end QPCs at low temperatures (\(< 4.2K\)) showed a splitting of the first conductance quantization plateau. The end QPCs are used as spin injectors and detectors with 100% efficiency to study spin-polarized transport in the central QPC. The 3-QPC device we have studied can conceivably be used to study Rashba spin precession in a 1D channel to check the concept of the Datta-Das spinFET.
4:30PM D12.00009 Spin Dynamics of InAs Quantum Dots with Uniform Height.1 2, T.A. KENNEDY, J. WHITAKER3, A.S. BRACKER, D. GAMMON, S.E. ECONOMOU, T.L. REINECKE, Naval Research Lab. — Spin splittings and relaxation times were studied by Time-Resolved Faraday Rotation (TRFR) in InAs self-assembled quantum dots. Three twenty-layer samples with different dopings were grown by the Indium-flush method. This technique produces a nearly constant dot-height of 2.5 nm. The TRFR was performed using a 1.3 ps pulse Ti:sapphire laser with the sample at 5.7 K. In the undoped and lightly doped samples, signals are observed from excitons in neutral dots and from electrons and trions in negatively charged dots. Simulations for both the neutral and charged dots account for the results very well. The in-plane electron g-factor is 0.42 and shows very little variation from sample to sample or with energy in spectral studies. We ascribe this to the fixed height of the dots. The hole g-factor can be extracted cleanly from the results for the heavily doped sample. Two of the samples exhibit mode-locking of the electrons spins at 12 ns demonstrating that T2 is much longer than T2*.

1Work supported in part by ONR.
2Now at ATK Thiokol, Brigham City, UT

4:42PM D12.00010 Gating a ferromagnetic semiconductor1, A. BOVE2, F. ALTMARE3, N. KUNDTZ, A.M. CHANG, Physics Department, Duke University, Durham, NC 27708, Y.J. CHO, X. LIU, J. FURDYNA, Physics Department, University of Notre Dame, Notre Dame, IN 46556 — Ferromagnetic semiconductors have the potential of revolutionizing the way current electronic devices work: more so, because they are compatible with current fabrication lines and can easily be integrated with today’s technology. Particular interest lies in III-V Diluted Magnetic Semiconductor (DMS), where the ferromagnetism is hole-mediated and the Curie temperature can therefore be tuned by changing the concentration of free carrier2. In these systems, most of the effort is currently applied toward the fabrication of devices working at room-temperature: this implies high carrier density accompanied by low mobility and short mean free path. We will report our results for a ferromagnetic 2DHG system with low carrier density (≈ 3.4×10^12 cm^-2) and mobility (≈ 1000 cm^2/(V*s)), and we will discuss the effects of local gating2 on light of possible applications to the fabrication of ferromagnetic quantum dots.

1Research supported in part by NSF NIRT DMR-0210519.
2Physics Department, Purdue University, West Lafayette, IN 47907
3Now at NIST, 325 Broadway, Boulder CO 80305

4:54PM D12.00011 Non-equilibrium Kondo effect in a quantum dot: Real-time density matrix formulation with non-crossing approximation , CHANGXUE DENG, XUEDONG HU, University of Maryland — We study the non-equilibrium electron transport through a quantum dot in the Kondo regime for an infinite-U Anderson model with the self-consistent non-crossing approximation (NCA). We apply the real-time density matrix (RTDM) formulation, which is appropriate for both equilibrium and non-equilibrium situations. We study the Kondo resonances by calculating the spectral function of the localized electron. Results are reported for both spin-degenerate and spin-resolved cases by applying external magnetic fields on the electron in the QD. It is well-known that NCA gives a spurious peak at the chemical potential as it neglect the vertex correction for the spin splitting case. We show that this spurious peak can be removed by using the exact result of the non-interacting Anderson model when calculating the empty state self-energy. We also discuss the differential conductance through the QD, which can be measured in a transport experiment. We find that the separation of the two Kondo peaks in the conductance for a spin resolved dot is smaller than twice of the Zeeman energy, and there exists a critical field below which the Kondo resonance does not split.

5:06PM D12.00012 Nuclear Polarisation in Quantum Wires . ANSON CHEUNG, Theory of Condensed Matter, Cavendish Laboratory, 19 J.J. Thomson Avenue, Cambridge CB3 0HE, UK, V. TRIPATHI, Department of Theoretical Physics, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai 400005, India — We consider the intriguing possibility that current flow within a quantum wire can produce nuclear polarization. The quantum wire is special because electrons can only move along one direction. Also, because of its heterogeneous structure, spin-orbit effects come into play. Together, this means that electrons are only permitted to have spin up or down orientations within the wire. By exploiting this and the Overhauser effect, we calculate the degree of nuclear polarization and the electronic conductance arising from the effect of a non-equilibrium current.

Monday, May 3, 2007 2:30PM - 5:06PM
 Session D13 DMP GMAG: Focus Session: Electronic Structures of Transition-Metal Oxides
 Colorado Convention Center Korbel 4C

2:30PM D13.00001 Probing the Electronic Structure of Metal Oxides using Resonant Inelastic Soft X-Ray Scattering and Soft X-ray Emission Spectroscopy.1 2, KEVIN E. SMITH, Boston University — While photoemission spectroscopy is often the probe of choice in studying the electronic structure of solids, there are many sample and environmental constraints that must be satisfied before meaningful data can be obtained with this spectroscopy. Specifically, samples generally need to be electrically conducting single crystals, with atomically clean and ordered surfaces. Clearly, complimentary electronic structure probes applicable to non-crystalline samples, insulators, or samples with poorly controlled surfaces are highly desirable. I will discuss the application of two such techniques: synchrotron radiation-excited soft x-ray emission spectroscopy and resonant inelastic x-ray scattering. By virtue of being photon-in/ photon-out probes, these techniques can measure the electronic structure with poorly controlled surfaces. Simulations for both the neutral and charged dots account for the results very well. The in-plane electron g-factor is 0.42 and shows very little variation from sample to sample or with energy in spectral studies. We ascribe this to the fixed height of the dots. The hole g-factor can be extracted cleanly from the results for the heavily doped sample. Two of the samples exhibit mode-locking of the electrons spins at 12 ns demonstrating that T2 is much longer than T2*.

1With: T. Learmonth, P.A. Glans, Y. Zhang (Boston U.); J. Guo (ALS); S. Hulbert (NSLS); D.J. Payne, R.G. Egdell (Oxford); A. Walsh, G.W. Watson, C. McGuinness (Trinity); A. Matsunara (AFOSR); J.E. Downes (Macquarie); and L.C. Duda, J. Nordgren (Uppsala).
3:06PM D13.00002 Hybridization of local Frenkel excitons in strongly interacting NiO

, WEI KU, CCMPSD, Brookhaven National Lab; Physics Department, State University of New York, Stony Brook, CHI-CHENG LEE, CCMPSD, Brookhaven National Lab; Physics Department, Tamkang University, Taiwan, R.O.C., HUNG-CHUNG J. HSEUH, Physics Department, Tamkang University, Taiwan, R.O.C. — Recent experimentally observed tightly bound excitons in NiO are explained by a newly developed linear response theory within LSDA+U approximation. A novel picture of local Frenkel excitons naturally emerges from a real space formulation of exciton formation using the energy-resolved Wannier functions. Systematic analysis of microscopic interacting processes reveals that the large 1 eV splitting between the excitons is due to a strong hybridization between the Frenkel excitons via strong local interactions. Our new picture can be viewed as a simplest representation of the charge excitation involving complex multiplet structure in strongly correlated systems.

3:18PM D13.00003 Unusual magnetic ground state in MnO under pressure, , KLAUS KOEPERNIK, IFW Dresden, Germany, DEEPA KASINATHAN, MPI-CPS, Dresden, Germany, WARREN E. PICKETT, Dept. of Physics, UC Davis, CA, USA — A study of the phase transitions in MnO under pressure is presented. The calculations are based on density functional theory. The onsite correlations in the Mn 3d shell are treated within the framework of LSDA+U. The major result is that the first phase transition (with increasing pressure), which is characterized by an isostructural magnetic moment collapse from spin $3/2$ to spin $1/2$, results in a low spin solution exhibiting an unexpected intra-atomic spin polarization pattern. An analysis of the influence of the symmetry, the magnetic ordering and the LSDA+U interactions shows that this unusual spin arrangement is the result of inter-atomic exchange terms. The dependence of the results on the parameters $U$ and $J$ will be discussed.

3:30PM D13.00004 Evolution of MnO under Pressure from Dynamical Mean Field Theory

, WARREN E. PICKETT, KWAN-WOO LEE, RICHARD T. SCALETAR, UC Davis, JAN KUNES, Univ. of Augsburg, A.V. LUKOYANOVA, Ural State Tech. Univ., Yekaterinburg, V.I. ANISIMOV, Inst. of Metal Physics, Yekaterinburg — Late transition metal oxides qualify as so called charge-transfer insulators whose description requires that the simple Hubbard interaction within the $3d$ orbitals has to be augmented by mixing with the ligand $2p$ states. MnO is a relatively simple realization (at ambient pressure) of such a system. Its pressure evolution at room temperature exhibits structural ($B1$B8), magnetic (high spin low spin) and electronic (insulator metal) transitions, and correlated band theories predict a $S=5/2$ to $S=1/2$ moment collapse. We report All-Electron + DMFT high-spin to low-spin or insulator to metal transitions, and a study of the paramagnetic fcc phase as volume is reduced, focusing on the behavior of the local magnetic moment and the metal-insulator transition. We also present single-particle excitation spectra that illuminate the character of the evolution.

3:42PM D13.00005 Structural and Electronic Properties of Monoclinic TiO$_2$ (B) Polymorph

, MICHEL POSTERNAK, ALFONSO BALDERESCHI, EPF-Lausanne, Switzerland, BERNARD DELLEY, Paul Scherrer Institut, Switzerland — Three major polymorphs of TiO$_2$ are known: rutile, anatase, and brookite. A further phase, TiO$_2$ (B), which coexists with, and derives from natural anatase has recently been identified. It is monoclinic with $C_{2h}^1$ space group, and its conventional cell contains 8 TiO$_2$ formula units. Using the DMol$^3$ approach we study the structural and electronic properties of this polymorph in terms of the OTI$_3$ complex, that we have recently shown to be the relevant building block for describing the electronic properties of the three major polymorphs. At variance with these latter cases, the 16 O atoms in TiO$_2$ (B) are not all threefold coordinated: indeed, 12 O atoms belong to anatase-like OTI$_3$ structural units, and the remaining 4 O atoms are twofold coordinated. The outcome of structural differences on the electronic properties of the TiO$_2$ phases is analyzed.

3:54PM D13.00006 Photoinduced charge and spin dynamics in strongly correlated electron systems

, HIROAKI MATSUEDA, SUMIO ISHIHARA, Tohoku University — It is widely recognized that the competition among multiple phases is a key issue to understand electronic properties in strongly correlated electron systems. A tiny amount of external perturbation breaks balance among these phases, and gigantic response appears. Photoirradiation by the femtosecond pulse laser is a powerful tool to induce the response. For understanding the mechanism of the response after the photoirradiation, pump-probe spectroscopy measurements on perovskite manganese oxides have been performed in recent years. The main issue is the photoinduced transition between ferromagnetic metallic and charge-ordered insulating (COI) phases. Motivated by the transition, we examine the effect of the photoirradiation on the COI phase in the extended double-exchange model. We calculate the transient optical absorption spectrum by the linear response theory within LSDA+U approximation. The major result is that the first phase transition (with increasing pressure), which is characterized by an isostructural magnetic moment collapse from spin $3/2$ to spin $1/2$, results in a low spin solution exhibiting an unexpected intra-atomic spin polarization pattern. An analysis of the influence of the symmetry, the magnetic ordering and the LSDA+U interactions shows that this unusual spin arrangement is the result of inter-atomic exchange terms. The dependence of the results on the parameters $U$ and $J$ will be discussed.

4:06PM D13.00007 Novel electronic and magnetic properties of a new class of cupper oxides

, XIAO HU, XIANGGANG WAN, MASANORI KOHNO, National Institute for Materials Science, Tsukuba 305-0047, Japan — Cuprates have not been considered seriously as candidate of useful magnetic material since the known ferromagnetic cuprates show quite low $T_C$. The recently reported cuprate Sr$_8$Ca$_6$Cu$_{24}$O$_{41}$, a Mott insulator with perovskite structure, exhibits surprisingly macroscopic magnetization up to $T_C = 440K$. Doing LSDA+ U calculations, we reveal theoretically that an orbital order appears in Cu atoms which results in a ferrimagnetic ground state, and that the p$^3$ d$^9$ bonds are responsible to the strong super exchange interactions and thus the high $T_C$. We propose a spin model and perform quantum Monte Carlo simulations, with which we can reproduce accurately the observed magnetization curve including the critical point $T_C$. Moreover, a half-metallic (HM), which behaves as metal for one spin channel and insulator for the opposite, is predicted when replacing Re with W or Mo. A novel picture of local Frenkel excitons naturally emerges from a real space formulation of exciton formation using the energy-resolved Wannier functions. Systematic analysis of microscopic interacting processes reveals that the large 1 eV splitting between the excitons is due to a strong hybridization between the Frenkel excitons via strong local interactions. Our new picture can be viewed as a simplest representation of the charge excitation involving complex multiplet structure in strongly correlated systems.
4:18PM D13.00008 Theory of thermopower in strongly correlated electron systems. WATARU KOSHIKABE, Sendai National College of Technology, SADAMICHI MAEKAWA, Institute for Materials Research, Tohoku University — We have studied the effects of spin and orbital degrees of freedom in the strongly correlated electron systems, and have derived the formula of the high-temperature thermopower:

\[ Q = -\left( k_B / e \right) \ln \left( g_e / g_h \right) - \left( k_B / e \right) \ln \left( n_b / \left( 1 - n_h \right) \right), \tag{1} \]

where \( n_b \) is the hole concentration, and \( g_e \) (\( g_h \)) denotes the local degeneracy of the electronic configuration on the transition metal ion without (with) hole carrier. The local degeneracy is determined by the spin and orbital degrees of freedom. It has been established that the formula (1) gives a good estimation of the thermopower in not only the 3d transition metal oxides but also the 4d ones, recently. We have studied the thermopower in the oxides composed of several kinds of transition metal ions. Its high-temperature formula shows a complicated expression, however, it is expressed to be the average of the first term of the equation (1) in the case that \( n_b = 0.5 \), in the double perovskite system. This is because the thermopower is nothing but the entropy carried by the electric current. We will discuss the thermopower of the oxides with several kinds of transition metal ions in the light of the theory.

4:30PM D13.00009 Hybrid density functional study of Mott transition in MnO. CRISTIAN V. DIACONU, RICHARD L. MARTIN, Los Alamos National Laboratory, IONUT D. PRODAN, GUSTAVO E. SCUSERIA, Rice University — The electronic structure, the magnetic moment and volume collapse of MnO under pressure is obtained from hybrid density functional theory using the recently developed screened hybrid exchange-correlation functional of Heyd, Scuseria and Ernzerhof (HSE). We study two crystal structures for MnO: cubic (rock salt) and hexagonal (nickel arsenide). We find two antiferromagnetic states for the NaCl structure: a high-spin state that couples two \( S = 5/2 \) moments, and a low-spin state that couples two \( S = 1/2 \) moments. At ambient pressure the high-spin state lies lowest. The low-spin phase is favored at a pressure of about 24 GPa, leading to a first order volume collapse. However, this transition is pre-empted by another first-order volume collapse at 17.1 GPa from the NaCl structure to a NiAs structure. This transition is predicted to be insulator to metal and is the realization of the Mott transition.

4:42PM D13.00010 Disorder driven quantum phase transitions in transition metal oxides. KOHIJIRO KOBAYASHI, NANDINI TRIVEDI, The Ohio State University — We investigate the effect of disorder on a class of transition metal oxides described by a single orbital Hubbard model at half filling and away from half filling. The phases are characterized by the nature of the electronic and spin excitations. We calculate the local density of states, frequency and temperature-dependent conductivity and spin susceptibility as functions of disorder and interaction. The interplay of disorder and correlations produces unusual behavior in the correlated metal, for example, characteristic suppression of density of states at low energies, persistence of gap like features at finite frequency and the presence of local moments. Some of these puzzles can be understood in terms of an inhomogeneous system composed essentially of two-components. We compare our results with recent local scanning tunneling spectroscopy, and optical conductivity measurements. Reference. De. Heidarian and N. Trivedi, Phys. Rev. Lett. 93, 166401 (2004); K. Kobayashi, B.H. Lee, and N. Trivedi, cond-mat.

4:54PM D13.00011 ABSTRACT WITHDRAWN —

Monday, March 5, 2007 2:30PM - 5:30PM — Session D16 DMP GMAG: Focus Session: Multiferroics II Colorado Convention Center Korbel 4F

2:30PM D16.00001 Manipulation of the ferromagnetic domains of a manganite using an electric field. TARA DHAKAL, SINAN SELCUK, ARTHUR F. HEBARD, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL — We have measured the response of the fluid like phases of ferromagnetic metal (FMM) and charge ordered insulator (COI) in thin films of the manganite \( \text{La}_{0.4} \text{Pr}_{0.6} \text{Ca}_{0.33} \text{MnO}_3 \) (LPCMO) to an external electric field. The electric field (set by applying a voltage difference across the material) alters the fluid phases and increases the conductivity of the material by about 2 orders of magnitude above a threshold voltage. To check if the enhanced conductivity is associated with an increase in the size of the FMM domains, we measured the magnetization of the thin films using a SQUID magnetometer with and without an applied electric field. The saturation magnetization remained the same in either case showing that the FMM domains do not increase in size, which led us to hypothesize that the domains are just reoriented by the electric field. This hypothesis was verified by measuring the transverse resistance while a voltage difference was applied longitudinally across the material. At a threshold voltage when the longitudinal resistance decreased by about 2 orders of magnitude, the transverse resistance showed a small increase. This increase in resistance was attributed to the FMM domains being stretched in the direction of the electric field.


2:42PM D16.00002 Controlling the magnetic phase of a hole-doped manganite with an out-of-plane electric field. SUNG HEE YUN, RAJIV MISRA, A. F. HEBARD, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL — We have measured the response of the fluid like phases of ferromagnetic metal (FMM) and charge ordered insulator (COI) in thin films of the manganite \( \text{La}_{0.4} \text{Pr}_{0.6} \text{Ca}_{0.33} \text{MnO}_3 \) (LPCMO) to an external electric field. The electric field (set by applying a voltage difference across the material) alters the fluid phases and increases the conductivity of the material by about 2 orders of magnitude above a threshold voltage. To check if the enhanced conductivity is associated with an increase in the size of the FMM domains, we measured the magnetization of the thin films using a SQUID magnetometer with and without an applied electric field. The saturation magnetization remained the same in either case showing that the FMM domains do not increase in size, which led us to hypothesize that the domains are just reoriented by the electric field. This hypothesis was verified by measuring the transverse resistance while a voltage difference was applied longitudinally across the material. At a threshold voltage when the longitudinal resistance decreased by about 2 orders of magnitude, the transverse resistance showed a small increase. This increase in resistance was attributed to the FMM domains being stretched in the direction of the electric field.


2:54PM D16.00003 Colossal piezoresistance in manganites. JACOB TOSADO, JOSYMIR LOPEZ, TARA DHAKAL, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL — We have studied the effect of the application of direct mechanical stress on thin films of the hole-doped manganite oxide (manganite) \( \text{La}_{0.4} \text{Pr}_{0.6} \text{Ca}_{0.33} \text{MnO}_3 \) (LPCMO). The two competing phases in manganites are the pseudocubic ferromagnetic metallic (FMM) phase and the orthorhombic charge-ordered insulating (COI) phase. Due to the different structures of the FMM and COI phases, manganites are susceptible to mechanical stress. The traditional methods of applying stress on oxide thin films result in different growth modes which makes it difficult to quantify the strain in the thin film. Using a calibrated screw we applied direct mechanical stress on the substrate and measured the change in the phase diagram of the manganite as a function of strain. Our results show that the effect of strain is the largest in the fluid phase separated region of the phase diagram, where we observe a strain-induced change in resistance of about 5 orders of magnitude.

[1] J. L. was supported by the REU program of the NSF at the Department of Physics, University of Florida.

3:06PM D16.00004 Spin filtering with magnetic oxide tunnel barriers, MANUEL BIBES, Insitut d Electronique Fondamentale, CNRS — Interesting physical phenomena and potential new devices arise when the barrier of magnetic tunnel junctions is made of a ferroic material. In the most studied case of magnetic barriers, carriers are spin-polarized by the spin-filter effect, which gives rise to tunnel magnetoresistance (TMR). We will present results on the use of ultrathin ferrimagnetic and ferromagnetic layers as tunnel barriers. We have use thin films of NiFe$_2$O$_4$ (NFO), $T_c$=850K, to filter electrons according to their spin with an efficiency of ~25%, as evidenced by a TMR of up to 60% in La$_2$Zr$_2$Ti$_2$O$_7$/MnO$_3$ (LSMO)/NFO/Au junctions. We will discuss these results in the frame of a model describing tunneling through epitaxial magnetic barriers. We will also show results on ferromagnetic films of BiMnO$_3$ and La$_2$Ce$_{1.1}$Bi$_{0.9}$O$_3$ (LBMO) and their use as spin-filter barriers. Interestingly, LBMO films are also ferroelectric and therefore exhibit a multiferroic character, that is retained down to thicknesses of only 2 nm. Accordingly, LSMO/LBMO/Au junctions exhibit four different resistance states, instead of two with conventional spin filters. We will discuss the origin of this behavior on the basis on the combination of the spin-filter effect and the influence of ferroelectricity on tunneling.

3:25PM D16.00007 Ferroelectricity in a Collinear Magnetic Phase of Orthorhombic Perovskites, IVAN SERGIENKO, Oak Ridge National Laboratory, CENR SEN, National High Magnetic Field Laboratory, ELBIO DAGOTTO, University of Tennessee and Oak Ridge National Laboratory — Below $T_c = 30$ K, a number of perovskite manganites (such as HoMnO$_3$) and nickelates order magnetically in the so-called E-type phase with zigzag chains of parallel spins. We demonstrate that this magnetic phase is also ferroelectric. We discuss the magneto-electric coupling based on the symmetry arguments of the Landau theory of phase transitions. We also explore a microscopic mechanism of ferroelectricity induced by the collinear spin arrangement and address the order of magnitude of the ferroelectric polarization.

3:35PM D16.00006 Ferroelectricity in perovskite HoMnO$_3$ and YMnO$_3$ induced by magnetic order, 1. B. LORENZ, Y. Q. WANG, C. W. CHU, 2. TCSUH and Dept. of Physics, University of Houston — Ferroelectricity is observed in orthorhombic HoMnO$_3$ and YMnO$_3$ at the magnetic lock–in transitions into an E-type structure or an incommensurate phase with a temperature independent wave vector, respectively. In HoMnO$_3$ the ferroelectric polarization strongly depends on the external magnetic field indicating the involvement of the rare earth moment order in this compound. The results are discussed within the framework of recent theoretical models, in particular the double exchange driven polar displacements predicted for E-type magnetic structures. The ferroelectric observed in YMnO$_3$ cannot be explained within the current picture of the magnetic order and a refinement of the magnetic structure seems to be necessary.

3:45PM D16.00008 Multiferroicity induced by phase modulated spin-density waves, JEROEN VANDENBRINK, Leiden University, JOSEPH BETOURAS, University of St. Andrews, GIANLUCA GIOVANNETTI, Leiden University — Materials in which magnetic and ferroelectric order coexist—termed multiferroics—have recently become the focus of much interest. From a technological point of view the possibility to control magnetic properties by electric fields and, vice versa, ferroelectric order by magnetic fields, is very attractive. But despite the possible coexistence of ferroelectricity and magnetism, materials with a pronounced interplay between these properties are very rare. Here we report on a novel route to generate such an interdependence: we show that symmetry arguments allow a finite magneto-electric coupling for any spin-density wave that is phase modulated and commensurate, even if the spin ordering is collinear. It is this new coupling that drives the formation of multiferroic phases at the magnetic commensurability transitions, for instance the one of YMnO$_3$ at 23 K. This example makes clear that materials with phase modulated spin-density wave ordering are a new class of multiferroics with a strong independance of magnetization and ferroelectric polarization.

4:30PM D16.00009 High Magnetic Tunability of Dielectric Properties in Magnetically-Driven Ferroelectricity, SANG-WOOK CHEONG, S. PARK, Y. J. CHOI, C. L. ZHANG, S. GUHA, Rutgers Center for Emergent Materials and Department of Physics & Astronomy, Rutgers, Piscataway, NJ 08854 — Lattice relaxation in magnetically-ordered states with broken inversion symmetry through exchange-striction can induce non-centrosymmetric lattice distortions, leading to the presence of electric polarization. In these magnetically-driven ferroelectrics, dielectric properties turn out to be highly susceptible to applied magnetic fields. Both symmetric and antisymmetric exchange coupling can be involved in the exchange-striction. Magnetically-driven ferroelectrics with the symmetric coupling are associated with antiferroelectric density wave (SDW) states, and the antisymmetric coupling, relevant to the Dzyaloshinskii-Moriya-type interaction, becomes active when ferroelectricity is induced by spiral magnetic orders. A few examples of magnetically-driven ferroelectrics, exhibiting high tunability of dielectric properties in magnetic fields, will be discussed.

4:42PM D16.00010 A Microscopic Model of Multiferroics RMn$_2$O$_5$, CHEN FANG, JIANGPING HU, Department of Physics, Purdue Univ. — A microscopic model is developed to explain the phase diagram and the mechanism of magneto-electro coupling in RMn$_2$O$_5$. We show that frustrated magnetic structure drives the system to a commensurate-incommensurate phase transition which can be understood as a competition between a collinear order, which stems from the ‘order by disorder’ mechanism, and a chiral symmetry order. The magneto-electric interaction couples the collinear order to the electric polarization. The low energy excitation and the effect of external magnetic field are also analyzed.

4:54PM D16.00011 Direct evidence of spin-phonon coupling in multiferroic DyMn$_2$O$_5$ via magneto-infrared measurements, 1. J. CAO, J. L. MUSFELDT, University of Tennessee, Y. J. WANG, National High Magnetic Field Laboratory, S. PARK, S.-W. CHEONG, Rutgers University — The infrared active phonons in multiferroic DyMn$_2$O$_5$ are investigated as a function of magnetic field and temperature. Both field-induced frequency shifts and oscillator strength redistributions are observed in three important modes (the f-manifold crystal field splitting of Dy$^{3+}$ near ~150 cm$^{-1}$, the Mn-O bending mode at ~270 cm$^{-1}$, and the Mn-O stretching mode near ~630 cm$^{-1}$), indicating strong spin-phonon coupling in this material. The crystal-field levels of Dy$^{3+}$ are weakly sensitive to temperature induced magnetic phase transitions, whereas the Mn-O bending and stretching modes are insensitive to these phase boundaries. These measurements provide direct proof of spin-lattice interactions in DyMn$_2$O$_5$.

1This work is supported by the U.S. Department of Energy.
5:06PM D16.00012 Magnetic-field-induced quantum phase transition in multiferroic BiMn$_2$O$_5$. J.W. KIM, S.Y. HAM, Y.S. OH, KEE ROON KIM, Seoul National University, S. PARK, S.-W. CHEONG, Rutgers University, P. SHARMA, M. JAIME, N. HARRISON, NHMFL-LANL. — Multiferroic BiMn$_2$O$_5$ exhibits both antiferromagnetic and ferroelectric ordering below ~40 K. We have systematically investigated the electric/magnetic phase of BiMn$_2$O$_5$ by magnetization (M), dielectric constant (e), electric polarization (P) and specific heat (C$_p$) measurements down to 0.6 K and magnetic field (H) up to 45 tesla. At 4 K, BiMn$_2$O$_5$ shows a single magnetic-field-induced transition near H$_c$ ∼18 T as evidenced by a sharp increase in M. Interestingly, e vs H shows a sharp peak at H$_c$, of which magnitude systematically increases as critical temperature $T_c$ approaches proximity to H$_c$. Furthermore, P changes its sign with increasing H from positive to negative near H$_c$ with no hysteresis. The trajectory of which above three transitions occur follows the scaling relation $T_c$(H)∼(H-H$_c$)$^{1/2}$. The shape of C$_p$ vs H curve indicates that this transition is 2nd order down to 0.6 K, consistent with the absence of hysteresis in M, e, and P measurements. Temperature dependent e measurements under fixed H near H$_c$ reveal that e increases on cooling to 5 K and slightly decreases down to 0.6 K, as similarly observed in a quantum paraelectric SrTiO$_3$. All of these observations support an interesting possibility that BiMn$_2$O$_5$ can be the first system to exhibit quantum fluctuation of ferroelectricity tuned by magnetic field.

5:18PM D16.00013 Local Structure of the Multiferroic System RMn$_2$O$_5$. T. A. TYSON, M. DELEON, Q. QIAN, NJIT, A. IGNATOV, CAMD, LSDU, S. PARK, S.-W. CHEONG, Rutgers U. — In order to understand the origin of the coupled magnetic and ferroelectric properties observed in RMn$_2$O$_5$, temperature and magnetic field dependent local structure measurements have been performed. The local structure about the rare earth (R) and the Mn sites have been examined. The atomic correlations involved in the spin-lattice coupling are identified. $^1$This work is supported by NSF DMR-0512196.

Monday, March 5, 2007 2:30PM - 5:30PM Session D20 DMP: Focus Session: Ferroelectric and Other Oxides Colorado Convention Center 105

2:30PM D20.00001 Electric Field Gradient Comparisons in Perovskites $^1$, DANDAN MAO, ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — Piezoelectric and dielectric properties of Pb-based complex ferroelectric alloys with the A(B'B''O$_3$)$_3$ perovskite structure depend on composition and the local ordering of the B-site cations. A prototypical example is Pb(Sb$_{1/3}$Ta$_{1/3}$)O$_3$ (PST), which is a normal ferroelectric when the B atoms are ordered and becomes a relaxor when they are disordered. Electric field gradients (EFG) are sensitive to variations in local structure, and they can be probed using high-field nuclear magnetic resonance experiments. Calculations of EFGs are presented using the LAPW method within the local density approximation. We examine trends in B-site EFGs as a function of composition and order in PST, Pb(Sc$_{1/3}$Ta$_{1/3}$)O$_3$ (PST), Pb(Sb$_{1/3}$Ta$_{1/3}$)O$_3$ (PSW), and Pb(M$_{1/3}$Nb$_{2/3}$)O$_3$ (PMN). We discuss these results in terms of B- and Pb-atom off-centerings, and B-atoms ordering.

$^1$Supported by ONR

2:42PM D20.00002 Comparative study of the properties of BaTiO$_3$ and PbTiO$_3$ using DFT (LDA, GGA), HF and hybrid (B3LYP) functionals , D. I. BILC, P. HERMET, PH. GHOSEZ, Departement de Physique, Universite de Liege, 4000 Liege, BELGIUM, J. INIGUEZ, Institut de Ciencia de Materials de Barcelona, 08193 Bellaterra, SPAIN — The study of ferroelectrics and ferromagnetics using Density Functional Theory (DFT) requires the use of density functionals with adjustable parameters. Among the most popular functionals are those of the Local Density Approximation (LDA), Generalized Gradient Approximation (GGA) and the hybrid functional B3LYP. In this work, we compare the properties of BaTiO$_3$ and PbTiO$_3$ calculated using LDA, GGA, HF and B3LYP. We find that the LDA and GGA give comparable results for the atomic distortions. However, full relaxation of the tetragonal phase using B3LYP gives a supertetragonality comparable to GGA. We performed hybrid calculations for different values of the three Becke’s parameters and found that the supertetragonality is introduced by the non-local part of the Becke GGA exchange. This suggests that a hybrid functional generated from a better GGA might provide simultaneously better structural and electronic properties of FE. 1. Z. G. Wu, and R. E. Cohen, PRB 73, 235116, (2006).

2:54PM D20.00003 Nuclear Magnetic Resonance Chemical Shielding Calculations of Bulk Oxides $^1$, DANIEL PECHKIS$^2$, ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — We will present calculations of nuclear magnetic resonance (NMR) chemical shielding in oxides, modeled using embedded clusters. NMR spectroscopy is an important probe of local structure in disordered materials, such as ferroelectric perovskite solid solutions. Combined with electric field gradient (EFG) calculations, a complete interpretation of high magnetic field NMR spectra is possible in principle. Determination of NMR parameters within the embedded cluster method allows the study of both periodic and disordered systems. Moreover, this approach can take advantage of mature chemical shielding methods found in standard quantum chemistry electronic structure packages at several levels of theory, including different forms of density functionals as well as more correlated approaches. Results will be presented for several materials including ferroelectric perovskites.

$^1$Supported by ONR
$^2$Partially Supported by a Virginia Space Grant Consortium Fellowship

3:06PM D20.00004 Structure and Antiferroelectric Properties of Cesium Niobate, Cs$_2$Nb$_4$O$_{11}$. JIANJUN LIU, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182 USA, ROBERT W. SMITH, Department of Chemistry, University of Nebraska at Omaha, Omaha, NE 68182 USA, CHUNJUA HU, Nebraska Center for Materials and Nanoscience, University of NebraskaLincoln, Lincoln, NE 68588 USA, KUAN-JIUH LIN, Department of Chemistry, Center of Nanoscience and Nanotechnology, National Chung-Hsing University, Taichung 402, Taiwan, Republic of China — We determined the crystal structure of Cs$_2$Nb$_4$O$_{11}$ by using single crystal X-ray diffraction. The structural refinements at both 100 and 297 K show it to have a centrosymmetric structure in point group mmm and orthorhombic space group Pnma. The lattice is comprised of niobium-centered tetrahedra and octahedra connected through shared vertices and edges: cesium atoms occupy channels afforded by the three-dimensional polyhedral network. We also studied the electric-field dependence of the polarization and observed double hysteresis loops which we interpret as the manifestation of antiferroelectricity. We then elucidated the origin of the antiferroelectricity by using symmetry analysis of the structural space groups.
3:18PM D20.00005 First-principles study of polarization and piezoelectric properties of Zn$_{1-x}$Mg$_x$O $^1$ — ANDREI MALASHCHEVICH, DAVID VANDERBILT, Rutgers University — Wurtzite ZnO can be substituted with up to ~30% MgO to form a metastable Zn$_{1-x}$Mg$_x$O alloy while still retaining the wurtzite structure. Because this alloy has a larger band gap than pure ZnO, Zn$_{1-x}$Mg$_x$O/ZnO quantum wells and superlattices have been much studied as promising candidates for applications in optoelectronic and electronic devices. Here, we report the results of an ab-initio study of the spontaneous polarization of Zn$_{1-x}$Mg$_x$O alloys as a function of their composition. We perform calculations of the crystal structure based on density-functional theory in the local-density approximation, and the polarization is calculated using the Berry-phase approach. We decompose the changes in polarization into purely electronic, lattice-displacement mediated, and strain mediated components, and quantify the relative importance of these contributions. We consider both free-stress and epitaxial-strain elastic boundary conditions, and show that our results can be fairly well reproduced by a simple model in which the piezoelectric response of pure ZnO is used to estimate the polarization change of the Zn$_{1-x}$Mg$_x$O alloy induced by epitaxial strain.

$^1$This work was supported by NSF Grant DMR-0549198

3:30PM D20.00006 Ferroelectricity in CsPbF$_3$ $^2$, MARCO FORNARI, Dept. of Physics, Central Michigan University — We discuss the structural and electronic features of ABX$_3$ halides with perovskitic structure. In particular we analyze the instabilities that drive CsPbF$_3$ to a rhombohedral phase and study the effect of halogen substitutions. The properties of CsPbF$_3$ are considered from the point of view of ferroelectricity and compared with prototypical oxides.

3:42PM D20.00007 Enhanced Piezoelectricity from Polarization Rotation in Perovskites $^3$, R.E. COHEN, Carnegie Institution of Washington — Theoretical and experimental studies show that the large electromechanical response of PbMg$_{1/3}$Nb$_{2/3}$O$_3$ (PMN)-PbTiO$_3$ (PT) and related perovskite materials is due to the ease of rotating the polarization with an electric field applied oblique to the polarization. The applied field rotates the polarization from a rhombohedral phase towards tetragonal through monoclinic. Underlying the large coupling is the large c/a strain (about 6%) of ferroelectric PT. The best materials, including the most commonly used piezoelectric material, PZT (PbZrO$_3$ (PZ)-PT) tend to be solid solutions with PT. The other endmember is typically a relaxor, such as PMN or PZT. Is the relaxor behavior crucial to obtaining large coupling transducer materials? First-principles total energy and linear response computations for PT show the surprising prediction of a pressure induced morphotropic phase transition from tetragonal to monoclinic to rhombohedral, and finally cubic. In the transition regions the dielectric constant and piezoelectric constants become very large, in fact larger than those of the new single crystal piezoelectrics PMN-PT and relatives. This shows that large strain piezoelectricity in solutions with PT is due to the behavior of PT itself, and the other components simply tune the transition to zero pressure. This suggests that the key to finding new materials is in finding new pure compounds with pressure induced morphotropic phase transitions. First-principles and multiscale simulations will be discussed for relaxor ferroelectrics. This work was done in collaboration with A. Asthagiri, Y. Lei, M. Sepliarsky., Z. Wu and X. Zeng.

$^2$Supported by the Office of Naval Research

4:18PM D20.00008 Theoretical study of ferroelectric KNO$_3$ $^4$, OSWALDO DIEGUEZ, Massachusetts Institute of Technology, DAVID VANDERBILT, Rutgers University — We present a detailed study of the structural behavior and polarization reversal mechanism in phase III of KNO$_3$, an unusual ferroelectric material in which the nitrate groups rotate during polarization reversal. This work extends a preliminary study presented as an example in our earlier paper on the mapping of the energy (E) versus polarization (P) in insulators$^5$. Here we analyze in detail a two-parameter model in which the energy of the system is written as a low-order expansion in the polarization and in the nitrate group orientation. Apart from confirming that this model reproduces very well the first-principles results for KNO$_3$ presented in Ref. [1], we construct its parameter-space phase diagram, and in particular we describe regions of parameter space in which the E(P) curves have an unusual triple-well structure. We also present first-principles calculations of KNO$_3$ under pressure, finding that as the material is compressed its E(P) curves change character, going from having continuous to having discontinuous first derivatives at zero polarization.


4:30PM D20.00009 Distortions in charge-ordered LuFe$_2$O$_4$ $^6$, TAKESHI NISHIMATSU, DAVID VANDERBILT, KARIN M. RABE, YOICHI HORIBE, SANG-WOOK CHEONG, Rutgers University, CLAUDE EDERER, Columbia University — Experimental evidence due to the behavior of PT itself, and the other components simply tune the transition to zero pressure. This suggests that the key to finding new materials is in finding new pure compounds with pressure induced morphotropic phase transitions. First-principles and multiscale simulations will be discussed for relaxor ferroelectrics. This work was done in collaboration with A. Asthagiri, Y. Lei, M. Sepliarsky., Z. Wu and X. Zeng.

$^1$Supported by the Office of Naval Research

4:42PM D20.00010 High-pressure x-ray diffraction of PbTiO$_3$ at low temperature, MUHTAR AHART, MADDURY SOMAYAZULU, RONALD COHEN, RUSSELL HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington — We combined the angular and energy dispersive x-ray diffraction methods to investigate the structural behaviors of PbTiO$_3$ (PT) in a diamond anvil cell (pressure up to 23 GPa) at 10 K. The energy dispersive x-ray diffraction results show drastic change in Bragg peak intensities at 16 and 20 GPa which indicate that lead titanate undergoes successive phase transitions with pressure. The results of angular dispersive x-ray diffraction indicate that the lattice parameters a and c decrease with pressure and increase with temperature at 10 and 11 GPa. Pressure induced phase transitions at low temperature are reversible. The experimental results confirm theoretical calculations, including the predicted phase diagram. This work is supported by the ONR under the contract number N000140210506 and the Carnegie/Department of Energy Alliance Center (CDAC) (DF-FC0300144).

4:54PM D20.00011 Phase diagram of PZT solid solutions near the morphotropic phase boundary from first principles, I. KORNEV, L. BELLAICHE, University of Arkansas, Fayetteville, Arkansas 72701, USA, P. E. JANOLIN, B. DKKHIL, Laboratoire Structures, Propreties et Modelisation des Solides, Ecole Centrale Paris, France, E. SUARD, Institut Laue-Langevin, Grenoble Cedex, France — A first-principles-derived scheme, that incorporates ferroelectric and antiferrodistortive degrees of freedom, is developed to study finite-temperature properties of Pb(Zr$_{1-\delta}$Ti$_\delta$)O$_3$ solid solutions near its morphotropic phase boundary $^1$. The use of this numerical technique (i) resolves controversies about the monoclinic ground-state for some Ti compositions, (ii) leads to the discovery of an overlooked phase, and (iii) yields three multiphase points, that are each associated with four phases. Additional neutron diffraction measurements strongly support some of these predictions. $^1$Igor A. Kornev, L. Bellaiche, P.-E. Janolin, B. Dkhil, and E. Suard, Phys. Rev. Lett. 97, 157601 (2006) This work is supported by ONR grants N00014-04-1-0413, N00014-01-1-0600 and N00014-01-1-0365, by NSF grant DMR-0404335, and by DOE grant DE-FG02-05ER46188.
5:06PM D2O.00012 Dynamic fluctuations and static speckle in critical X-ray scattering from SrTiO$_3$, MARTIN HOLT, Argonne National Laboratory, MARK SUTTON, McGill University, PAUL ZSCHACK, HAWOONG HONG, Argonne National Laboratory, T.-C. CHIANG, University of Illinois at Urbana-Champaign — We report a study of critical x-ray scattering from SrTiO$_3$ near the antiferrodistortive structural phase transition at $T_C \approx 105$K. A lineshape analysis of the thermal diffuse scattering results in the most precise experimental determination to date of the critical exponent $\gamma = 1.38 \pm 0.08$. The microscopic mechanism behind the anomalous “central peak” critical scattering component is clarified here by the first-ever observation of a static coherent diffraction pattern (speckle pattern) within the anomalous critical scattering of SrTiO$_3$. This observation allows us to directly attribute the origins of the central peak to Bragg diffraction from remnant static disorder above $T_C$.

5:18PM D2O.00013 Theoretical investigation of phase transitions in hafnia, XUHUI LUO, ALEXANDER A. DEMKOV, The University of Texas — Transition metal (TM) oxides find applications in ceramics, catalysis and semiconductor technology. In particular, hafnium dioxide or hafnia will succeed silica as a gate dielectric in advanced CMOS devices. However, the thermodynamics properties of thin TM oxide films are not well understood, despite their technological importance. We study theoretically phase transitions in hafnia using density functional theory. We find that the cubic phase of hafnia transforms without a barrier into a tetragonal phase via a soft-phonon mode. The direct calculation of the cubic phase phonon dispersion confirms the existence of a zone edge soft mode in the cubic phase. We study the nxed elastic band method (NEBM) we find a barrierless transition path between the cubic and tetragonal phases which coincides with the same soft-mode path. In addition we identify the pathway for the tetragonal to monoclinic phase transition, and find a 0.045 eV/mol barrier. We construct the effective Hamiltonian for zone center distortions correct to the fourth order including the strain renormalization. The energy surface found correctly explains the symmetry of the phase structure observed at low temperature. We find that there are two sides to the phase transition driving forces. First there are local distortion modes; secondly there is strong coupling between the local modes. The coupling determines the transition temperature. We calculate the coupling and estimate the 3-D cubic to tetragonal transition temperature in fair agreement with experiment.

Monday, March 5, 2007 2:30PM - 5:30PM –
Session D22 GSNP DMP: Focus Session: Fracture —
Colorado Convention Center 108

2:30PM D22.00001 Failure of heterogeneous materials: Scaling properties of fracture surfaces and implications on models of cracks in disordered media. — DANIEL BONAMY$^1$, Groupe Fracture DMS/DRECAM/SPCSI CEA Saclay — While there exists a unified theoretical framework - Linear Elastic Fracture Mechanics (LEFM) - to describe the failure of homogeneous materials, understanding and modelling the mechanical properties of heterogeneous media continue to raise significant fundamental challenges. These mechanical properties, observed at the macroscopic scale, result from microscopic processes occurring at the scale of the material. To include these local processes into a statistical description constitutes then a crucial step toward the setup of predictive macroscopic models. Crack surface roughness is a consequence of these local processes. Consequently, many fracture experiments have focussed on their analysis. In this context, it was recently evidenced that, in many materials, fracture surfaces exhibit anisotropic scaling properties reminiscent to interface growth problems, fully characterized by two couples of parameters: The roughness exponents and the characteristic length-scales measured along and perpendicular to the direction of crack growth respectively. While the characteristic length-scales do depend on the considered material, the exponents are surprisingly universal: Two distinct sets of critical exponents are observed whether the surfaces are examined at scales below or above the size of the damaged zone at the crack front. Models of crack growth in disordered media are discussed at the light of these experimental observations. In particular, one can derive a model from LEFM which describe the development of crack roughness as an “elastic” manifold creeping in a random media. This approach captures quantitatively the experimental observations performed at length-scales above the size of the process zone. In this approach, the onset of crack propagation can be interpreted as a dynamic phase transition while sub-critical crack growth can be assimilated to thermally-assisted depinning.

$^1$with Laurent PONSON, Elisabeth BOUCHAUD, Harold AURADOU, Jean-Pierre HULIN

3:06PM D22.00002 Low self-affine exponents of fractured glass ceramics surfaces. — LAURENT PONSON, Federal University of Rio de Janeiro, HAROLD AURADOU, FAST-Univrsite Paris-Sud, DANIEL BONAMY, ELISABETH BOUCHAUD, SPCSI-Commissariat a l’Energie Atomique, JEAN-PIERRE HULIN, FAST- Universite Paris-Sud, FRACTURE GROUP TEAM, MELANGE ET MILIEUX DISPERSES TEAM — The morphology of fracture surfaces encodes the various complex damage and fracture processes occurring at the microstructure scale during crack propagation. It is now well established that fracture surfaces are self-affine characterized by a roughness exponent usually found close to $\zeta \approx 0.75$ for a wide range of materials. Recently, fracture surfaces of sandstone were found to be also self-affine but with a lower roughness exponent $\zeta \approx 0.4-0.5$. To investigate its origin, we studied fracture surfaces of glassy ceramics which are obtained by sintering glass beads. Such a material mimics the structure of sandstone with the advantage that their porosity may be tuned. They are also found to be self-affine, characterized by a roughness exponent $\zeta \approx 0.40 \pm 0.04$ significantly lower than the “universal” roughness exponent $\zeta \approx 0.75$ widely reported in the literature. Its value is found to depend very slightly on the crack growth velocity and the microstructure (grain diameter, porosity) in the range studied. This suggests the existence of a second universality class in failure problems. Its physical origin is then discussed and a model proposed.

3:18PM D22.00003 Rapid and slow self-affine fracture in glass. — MOISES HINOJOSA, FIME-UANL, CLAUDIA GUERRA, DSM/DRECAM/SPCSI, France. LEONARDO CHAVEZ, EDGAR REYES-MELO, VIRGILIO GONZALEZ, FIME-UANL, PROGRAMA DOCTORAL EN INGENIERIA DE MATERIALES, FIME-UANL, MEXICO. TEAM, FRACTURE GROUP, SERVICE DE PHYSIQUE ET CHIMIE DES SURFACES ET INTERFACES, DSM/DRECAM/SPCSI, FRANCE. TEAM — We discuss the self-affine properties of the fracture surfaces of soda-lime glass obtained in conditions of both rapid and slow fracture in bending. The fracture surfaces were studied by SEM and AFM. The analysis of the mirror and mist-hackle zones for the two conditions suggest the existence of two well defined self-affine regimes governed by universal or attractor values. At low-speed/finite-scales the roughness exponent $\zeta = 0.5$. $\zeta$ dominates whereas the value $\zeta = 0.8$ is recovered for high-speed/large scales regimes. These values are subjected to significant deviations that give rise to a possible transitional regime at intermediate scales and speeds, where both attractor values may coexist, particularly in the case of slow fracture. In this context the transitional regime can thus be regarded as the result of the competition of these attractors at intermediate scales and velocities.

3:30PM D22.00004 Roughness Exponent Measurements for the Central Force Model. — JAN Ø. H. BAKKE, ALEX HANSEN, Department of Physics, NTNU, Trondheim, Norway — We study the roughness properties of fracture profiles from the two-dimensional central force lattice model for a wide range of disorders. The intrinsic and the extrinsic roughness exponent have been measured together with the step size distribution $p(l)$. We find that the profiles are self-affine for systems with narrow disorders and that broader disorders introduces overhangs in the fracture surface leading to deviation from self-affinity for small length scales and to non-trivial finite size scaling.
3:42PM D22.00005 Local waiting time fluctuations along a randomly pinned crack front

STEPHANE SANTUCCI, KNUT JORGEN MALOY, RENAUD TOUSSAINT, JEAN SCHMITTBULH, University of Oslo — The propagation of an interfacial crack along a heterogeneous weak plane of a transparent Plexiglas block is followed using a high resolution fast camera. We show that the fracture front dynamics is governed by local and irregular avalanches with very large size and velocity fluctuations. We characterize the intermittent dynamics observed, i.e. the local pinnings and depinnings of the crack front which trigger a rich burst activity, by measuring the local waiting time fluctuations along the crack front during its propagation. The local front line velocity distribution deduced from the waiting time analysis exhibits a power law behavior, \( P(v) \propto v^{-\gamma} \) with \( \gamma = 2.55 \pm 0.15 \), for velocities \( v \) larger than the average front speed \( \langle v \rangle \). The burst size distribution is also a power law, \( P(S) \propto S^{-\eta} \) with \( \eta = 1.7 \pm 0.1 \). Above a characteristic length scale of disorder \( L_d \sim 20 \mu m \), the avalanche clusters become anisotropic, and the scaling of the anisotropy ratio provides an estimate of a local roughness exponent, \( H = 0.6 \).

3:54PM D22.00006 A Dissipative Particle Dynamics Model of Fracture

P.-P. CORTET, S.G. ROUX, S. CILIBERTO, Laboratoire de Physique, ENS Lyon, France — We present experiments on the slow growth of a single crack in a paper sheet submitted to a constant force \( F \). The non-averaged crack growth curves present a stepwise growth dynamics. Modelling the material as a lattice where the crack is pinned by elastic traps and grows due to thermal noise, we find that, in agreement with experiments, the distribution of step sizes follows subcritical point statistics with a power law (exponent 3/2) and a stress-dependent exponential cutoff diverging at the critical rupture threshold [1]. Taking into account the microstructure of cellulose fibers, the model is able to reproduce the shape of the statistically averaged crack growth curves, the dependence of the characteristic growth length on \( F \) as well as the effect of temperature on the rupture time. Finally, roughness of the crack interface is shown to depend on whether the crack grows in the subcritical regime, or in the rapid regime, over the critical rupture threshold. We analyze this roughness difference using a new approach based on the cumulants of the statistical distribution of the crack front height variations.


4:06PM D22.00007 Sub-critical crack growth in a sheet of paper

L. VANEL, S. SANTUCCI, N. MALLICK, P.-P. CORTET, S.G. ROUX, S. CILIBERTO, Laboratoire de Physique, ENS Lyon, France — We present experiments on the slow growth of a single crack in a paper sheet submitted to a constant force \( F \). The non-averaged crack growth curves present a stepwise growth dynamics. Modelling the material as a lattice where the crack is pinned by elastic traps and grows due to thermal noise, we find that, in agreement with experiments, the distribution of step sizes follows subcritical point statistics with a power law (exponent 3/2) and a stress-dependent exponential cutoff diverging at the critical rupture threshold [1]. Taking into account the microstructure of cellulose fibers, the model is able to reproduce the shape of the statistically averaged crack growth curves, the dependence of the characteristic growth length on \( F \) as well as the effect of temperature on the rupture time. Finally, roughness of the crack interface is shown to depend on whether the crack grows in the subcritical regime, or in the rapid regime, over the critical rupture threshold. We analyze this roughness difference using a new approach based on the cumulants of the statistical distribution of the crack front height variations.

This work was funded by ANR grant 05-JCJC-0121-01.

4:18PM D22.00008 Stability and roughness of crack paths in 2D heterogeneous brittle materials

EYTAN KATZAV, MOKHTAR ADDA-BEDIA, BERNARD DERRIDA, LPS - Ecole Normale Superieure, Paris — We present a recent study on the stability of propagating cracks in heterogeneous two-dimensional brittle materials and on the roughness of the surfaces created by this irreversible process. We introduce a stochastic model describing the propagation of the crack tip based on an elastostatic description of crack growth in the framework of linear elastic fracture mechanics. The model recovers the stability of straight cracks and allows for the study of the roughening of fracture surfaces. We show that in a certain limit, the problem becomes exactly solvable and yields analytic predictions for the power spectrum of the paths. This result suggests a surprising alternative to the conventional power law analysis often used in the analysis of experimental data and thus calls for a revised interpretation of the experimental results.

4:30PM D22.00009 Statistical properties of microcracking in polyurethane foams under tensile and creep tests: influence of temperature and density.

STEPHANIE DESCHANEL, GERARD VIGIER, NATHALIE GODIN, GEMPPM, INSA Lyon, France, LOIC VANEL, SERGIO CILIBERTO, Laboratoire de Physique, ENS Lyon, France — For some heterogeneous materials fracture can be described as a clustering of microcracks: global rupture being not controlled by a single event. We focus on polyurethane foams whose heterogeneities (pores) constitute the termination points where microcracks can stop. We record both the spatial and time distributions of acoustic emission emitted by a sample during mechanical tests: each microcrack nucleation corresponds to a burst of energy that can be localized on the widest face of the specimen. The probability distributions of the energy released is power-law distributed, independently of the material density, the loading mode or the mechanical behavior. On the other hand, the agreement of a power law for the time intervals between two damaging events seems to require a quasi constant stress during damaging. Moreover, we notice a behavior difference of the cumulative number of events and the cumulative energy of the localized events with temperature in the case of tensile tests and not any more for creep tests. The occurrence of a unique behavior and a power law in a restricted time interval for the cumulative number of events and the cumulative energy in creep allow us to apprehend interesting later studies of materials’ lifetime prediction.

4:42PM D22.00010 Do Plastic Zones form at Crack Tips in Silicate Glasses?

THEO FETT, JEAN-PIERRE GUIN — In a number of recent studies, the claim has been made that silicate glasses fracture by the formation, growth and coalescence of cavities, in the same way as in metals but at a much smaller scale. Evidence for this premise is based on the examination of side surfaces of fracture mechanics specimens, at the point where the crack intersects the free surface. Such measurements were carried out with an atomic force microscope, which demonstrated finite depressions in the regions around and in front of crack tips in silicate glasses. The height profile around crack tips supposedly differed from that obtained from a simple linear elastic fracture mechanics analysis; while, in front of the crack tip small depressions were observed which were interpreted as cavities. We used a three-dimensional finite element analysis to show that the calculated depression around the crack tip is in excellent agreement with that obtained by atomic force microscopy. In addition, we used AFM measurements on the fracture surfaces themselves to demonstrate the absence of the kind of residual damage that should be present on fracture surfaces if cavitation occurred at crack tips in glass. Our results are proof that cracks in glass propagate by brittle fracture; glass is elastic and bond snapping is the dominant feature of crack growth.

4:54PM D22.00011 Fragmentation in brittle rods

NICOLAS VANDENBERGHE, ROMAIN VERMOREL, EMMANUEL VILLERMAUX, IRPHE, Aix-Marseille Université — When a rod made of brittle material is axially impacted it breaks into fragments of various sizes. Before the first breaking event, an axial compression wave propagates along the rod, triggering a buckling instability. The instability selects a transverse mode with a well defined wavelength. Recently, Gladden et al. have shown that the fragment size distribution exhibits two peaks corresponding to the length selected by the buckling instability. In the present work we explore in more details the dynamics of elastic waves in the rod and the different phenomena that may explain the broad distribution of fragment sizes. In particular, we will discuss the coupling between the longitudinal and the transverse displacement in the post buckling dynamics.
The fracture process is usually analyzed in terms of the fractal dimension of a crack, the crack surface roughness, or fragment size distributions. It is established that relatively simple scaling laws exist for the crack surface roughness in model I fracture and for the power law distribution for fragment sizes in fracture by impact. These two types of fracture are usually studied separately. Consequently, much less is known about the relationship between crack roughness and fragment size distribution. In this work, we study this relationship by developing a simple model of model I fracture, which nevertheless provides sufficiently rich behavior in terms of crack roughness and fragment formation. Using this model, we show that different roughness in local regions of the crack path leads to different mechanisms for the subsequent fracture of those regions. We observe two robust power laws for the size distribution of smaller and larger fractures. We connect measurements in fragment size distribution with the local fractal dimension of cracks in the region of fragment formation.

Monday, March 5, 2007 2:30PM - 4:54PM
Session D23 DMP DCOMP: Focus Session: High Pressure III - Earth and Planetary Materials
Colorado Convention Center 110

2:30PM D23.00001 First principles investigation of the ice VII-VIII (order-disorder) phase boundary1 
RENATA WENTZCOVITCH, KOICHIRO UMEMOTO, MSI and CEMS, University of Minnesota, STEFANO DE GIRONCOLI, STEFANO BARONI, SISSA and DEMOCRITOS National Simulation Center, Trieste, Italy — Phase boundaries among the various forms of ice are difficult to determine experimentally because of the large hystereses involved. Theoretical determination is also very challenging. Treatment of disorder in hydrogen sublattice is one of major problems. We present a first-principles study of order-disorder transition between ice VII and VIII. This study involves the complete statistical sampling of configurations generated within a 16 molecules supercell and includes the important effects of vibrational energy on this phase boundary. Since this transition has been well constrained experimentally, it is a good test of our treatment.

1Research supported by NSF/EAR 013533, 0230319, and NSF/ITR 0428774 (VLab). Computations were performed at the Minnesota Supercomputing Institute.

2:42PM D23.00002 Freezing kinetics in overcompressed water1 
MARINA BASTEA, S. BASTEA, J. REAUGH, D. REISMAN, Lawrence Livermore National Laboratory — The transformation of water into ice is among the most common first order phase transitions occurring in nature, but it is far from being an ordinary one. Water has unusual physical properties both as a liquid and as a solid due largely to hydrogen bonding effects, which also play a major role in determining the characteristics of its freezing kinetics. We report high pressure dynamic compression experiments of liquid water along a quasi-adiabatic path leading to the formation of ice VII. We observe dynamic features resembling Van der Waals loops and find that liquid water is compressed to a high pressure state close to the ice density before the onset of crystallization. By analyzing the characteristic kinetic time scale involved we estimate the nucleation barrier and conclude that liquid water has been compressed to a high pressure state close to its thermodynamic stability limit.

1This work was performed under the auspices of the U. S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

2:54PM D23.00003 The effect of dynamic compression on phase transformation: Solidification of water and crystal growth of ice VI using dynamic diamond anvil cell1 
GEUN WOO LEE, WILLIAM EVANS, CHOONG-SHIK YOO, Lawrence Livermore National Laboratory — The kinetics of phase transformation depends on how driving parameters are applied. Under high pressure, compression rate can give different paths of phase transformation. For this purpose, we have developed a new device, called dynamic diamond anvil cell (d-DAC), which can modulate a given static pressure with various compression rate and type. Using d-DAC, liquid water can be overpressurized up to 75% in ice VI phase field without crystallization, and after transforms to metastable iceVII phase in the stable ice VI pressure field. Interestingly, when fast sinuosidal compression is applied, the crystal morphology of ice VI surrounded by liquid water dramatically changes to fractal and dendritic shape. In this talk, we will describe the details of crystallization, following a brief description of the technical development of d-DAC.

1This work was supported by PDRP under the auspices of the U. S. DOE by University of California, LLNL under Contract No. W-7405-Eng-48.

3:06PM D23.00004 Laser-driven shock studies on planetary ices 
KANANI LEE, New Mexico State University — Planetary ices such as water, methane and ammonia make up the bulk composition of planets such as Uranus and Neptune. Additionally, extra-solar planets recently discovered may also be partially composed of these ices. Due to their shear size, the interiors of these planets are at simultaneous high pressures and temperatures. Using laser-driven shock compression, experiments at these extreme conditions—up to ~10 TPa pressures currently and up to ~100 TPa (1 Gbar) in the near future—is possible and covers the full range of planetary pressures, including “super-giant” extra-solar planets. Additionally we can couple the dynamic compression with that of static compression in a diamond-anvil cell in order to decrease the temperatures along the principal Hugoniot. Laser-driven shock compression of water samples pre-compressed to 1 GPa produces high-pressure and high-temperature conditions inducing two significant changes in the optical properties of water: the onset of opacity followed by enhanced reflectivity in the initially transparent water. The onset of reflectivity at infrared wavelengths can be interpreted as a semi-conductor → electronic conductor transition in water, and is found at pressures above ~130 GPa for single-shocked samples pre-compressed to 1 GPa in contrast to pressures above ~100 GPa for water samples without precompression. Our results indicate that conductivity in the deep interior of “icy” giant planets is greater than realized previously because of an additional contribution from electrons.

3:42PM D23.00005 ABSTRACT WITHDRAWN —
3:54PM D23.00006 High pressure-temperature Raman spectroscopy of H2–H2O clathrate. MADDURY SOMAYAZULU, Geophysical Laboratory, Carnegie Institution of Washington, ALEXANDER LEVEDAHL, St. Anselm’s Abbey School, ALEXANDER GONCHAROV, HO-KWANG MAO, RUSSELL HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington — The melting curve of the C2 clathrate H2–H2O has been determined by in-situ Raman spectroscopy measurements in an externally heated diamond anvil cell. We have determined the melting curve to a maximum pressure of 27 GPa. These are the first measurements on the melting line in this clathrate. Depending on the stoichiometry of the starting mixture of H2 and H2O, we are able to study either a mixture of C2 and H2O or C2 and H2. In either case, we were able to pinpoint the melting of the clathrate from the measurements of the molecular stretching mode (vibron) in the clathrate. In the case of C2 + H2, we observe the vibron in the clathrate at a frequency higher than in pure H2 at the same pressure. We have cross-calibrated the melting temperatures using the Stokes-anti Stokes ratio of the diamond first order and Raman active TO phonon of cubic Boron Nitride. We find that the clathrate melts well above the H2 melting at all pressures studied indicating that the stabilization of this clathrate at high pressures is indeed due to interactions between the host and guest molecules.

4:06PM D23.00007 Computational analysis of methane occupation within gas hydrates. PHILLIP MENDONCA, PHILIP SHEMELLA, SHAROJ NAVAY, Department of Physics, Applied Physics, and Astronomy. Rensselaer Polytechnic Institute, ANURAG SHARMA, Department of Earth and Environmental Sciences. Rensselaer Polytechnic Institute — Gas hydrates are considered a future energy resource that have large quantities of hydrocarbon gases (mostly methane) trapped and stabilized under moderate pressures in continental shelf and permafrost regions. The global estimate of hydrocarbon stored in these ice-like structures far exceeds all fossil fuel reserves. Methane escape from these phases, therefore, is considered a potential global warming contributor. These characteristics make the gas hydrates energy recovery a technological challenge and requires constraining the methane diffusion process within the structure. Here, we present a first principles theoretical investigation into the structure, energetics and dynamics of the “guest” molecule in gas hydrates, with the goal of building a physical model for methane diffusion. In particular, our study focuses on the sI (low pressure) methane hydrate phase by combining isolated cluster calculations and periodic structure calculations and closely guided by high pressure experimental work on methane hydrate. Based on the known crystal structure, we compare binding energies for methane and other gas molecules (e.g. Xe, Ar, CO2) to guide the high pressure experiments.

4:18PM D23.00008 Theoretical Tools for the Analysis and Prediction of Multi-component Systems at High Pressures and Densities. J. F. KENNEY, A.P.S. — J. F. Kenney, Gas Resources Corporation, Houston, Texas, U.S.A. To describe or predict theoretically the evolution of a multi-component system at high pressures, one must have a reliable expression for the system’s partition function, or its Helmholtz free energy, or its equation of state. Such formalism must possess the following properties: The formalism must be based upon fundamental, first-principles, quantum statistical mechanics argument, and the highest level of rigor available; it cannot be

4:30PM D23.00009 The Modern Theory of Abiotic Deep Genesis of Hydrocarbons: Experimental Confirmation. VLADIMIR KUTCHEROV, Prof. — The concept of the abiotic deep genesis of hydrocarbons, developing during the last 50 years in Russia, recognizes petroleum as a primordial material of deep origin erupted into the crust of the Earth. Until recently, this concept was a geologists’ hypothesis. Now, theoretical arguments and experimental results place the modern theory of the abiotic deep genesis of hydrocarbons in the mainstream of modern thermodynamics, experimental physics and physical chemistry. Recent experimental results confirm the possibility of hydrocarbon synthesis under conditions of the upper mantle. The mixture of the hydrocarbons has been obtained as a result of chemical reactions in the system CaCO3-H2O-FeO at pressures of 3-5 kbar and at temperatures of 1200-1500 K. Two different paths of hydrocarbons synthesis were detected using X-ray, mass-spectrometer and chromatograph analysis. These experimental demonstrations of the spontaneous, high-pressure genesis of hydrocarbons can be accepted as partial proof of the modern theory of petroleum. Modern Russian petroleum science allows application of a new approach to methods for petroleum exploration, oil and gas formation, and to reexamine the world’s hydrocarbons reserves.

4:42PM D23.00010 Chemical Dissociation of Cyclohexane under Shock Loading. RICKY CHAU, NEIL C. HOLMES, Lawrence Livermore National Laboratory — We present a study of the chemical dissociation process in the ringed hydrocarbon cyclohexane under shock loading. Cyclohexane was subjected to shock loading in the pressure range of 12 GPa to 39 GPa. The dissociation was observed using double pass optical absorption spectroscopy. We observed the onset of dissociation as the shock pressure was increased. A strong wavelength dependence was observed in the absorption first beginning at 650 nm and eventually at 400 nm at 39 GPa. The absorption mechanism is is suggestive of Mie scattering of fine carbon particles. The kinetics of the dissociation and the formation of the carbon particles will be discussed.

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

Monday, March 5, 2007 2:30PM - 5:30PM – Session D28 DMP: Focus Session: Carbon Nanotube Optics II Colorado Convention Center 302

2:30PM D28.00001 Inelastic X-ray Scattering Studies of Plasmons in Carbon Nanotubes1. M.H. UPTON, R.F. Klie, J.P. Hill, Brookhaven National Laboratory, T. GOG, D. CASA, Advanced Photon Source, Argonne National Laboratory, W. KU, Y. ZHU, M.Y. SFEIR, J. MISEWICH, Brookhaven National Laboratory, G. ERES, D. LOWNDES, Oak Ridge National Laboratory — We investigate the physical parameters controlling the low energy screening in carbon nanotubes via electron energy loss spectroscopy and inelastic x-ray scattering. Two plasmon-like features are observed, one near 9 eV (the so-called π plasmon) and one near 20 eV (the so-called π + σ plasmon). At large nanotube diameters, the π + σ plasmon energies depend exclusively on the number of walls and not on the radius or chiral vector. This shift indicates a change of strength of screening and the effective interaction at inter-atomic distance, and thus suggests an alternative mechanism of tuning the properties of the nanotube in addition to the well-known control provided by chirality and tube diameter.

1Work performed at BNL, the Advanced Photon Source and ORNL was supported by the US DOE under contracts No. DE-AC02-98CH10886, No. W-31-109-Eng-38 and DE-AC05-00OR22725 respectively.
2:42PM D28.00002 Ab-initio study of metallic and semi-metallic carbon nanotubes . . . SUMIT SAXENA, TREVOR A. TYSON, New Jersey Institute of Technology - Newark — We present first principle calculations to study the metal – semiconductor transitions with pressure in zigzag nanotubes using the Local density approximation. Spin restricted calculations for metallic (9, 0) and semi-conducting (10, 0) carbon nanotubes were performed using the full potential projected augmented wave (PAW) method and using ultra-soft pseudo potentials. Our calculations show qualitative agreement to the reported experimental density of states (DOS) for the semi-conducting (10, 0) nanotubes [1]. The band gap between the valence and the conduction band using the pseudo potential formalism is found to be very close to that predicted using PAW approach. We observe that the DOS obtained using pseudo potentials reproduce the essential features however the full potential approach reproduces most of the features of the experimentally reported results. The details of the calculations and other results will be presented. [1] T. W. Odom, J. L. Huang, P. Kim, C. M. Lieber, J. Phys. Chem. B 104 2794 (2000)

2:54PM D28.00003 Raman Study of Phonon Softening in Individual Metallic Single Wall Nanotubes , HOOTAN FARHAT, HYUNGBIN SON, JING KONG, MIT — We have studied the Breit-Wigner-Fano (BWF) lineshape and frequency of the G band in individual metallic nanotubes as function of the Fermi level position. Single wall carbon nanotubes are grown from dispersed nanoparticles and are doped electrostatically by means of a polymer electrolyte gate. The frequency of the G phonon in metallic tubes is very sensitive to the position of the Fermi level. As the Fermi level is tuned below and above the Fermi point, a semiconducting like G-band is recovered both in terms of frequency and linewidth. Near the Fermi point, the downshift of the G` frequency with respect to that of semiconducting tubes reaches a maximum of up to 50 cm$^{-1}$. The doping and diameter dependence of the phonon softening are explained in terms of electron phonon coupling.

3:06PM D28.00004 Controlled Screening of Excitons in Single, Suspended Carbon Nanotubes . , ANDREW WALSH, Physics Dept., BU, A. NICKOLAS VAMIVAKAS, ECE Dept., BU, YAN YIN, Physics Dept., BU, STEPHEN CRONIN, EE Dept., USC, BENNETT GOLDBERG, Physics Dept., BU, M. SELIM UNLU, ANNA SWAN, ECE Dept., BU — Recent measurements in carbon nanotubes (CNTs) have demonstrated that the optical transition energies are excitonic (e-h) in nature, with binding energies that are large fractions of an eV. The exciton energies in CNTs should be sensitive to screening by the environment, yet only small variations of the optical transition energies have been reported for widely varying dielectric environments. Here, we use resonant Raman spectroscopy to follow the change in the optical transition energy of single carbon nanotubes suspended across trenches in dry nitrogen, in high humidity, and after immersion in water. The transition energies are shown to red shift monotonically with increased screening, up to 33 meV. We develop a scaling relationship between the exciton binding energy and the external electric field due to screening, and show that this relationship can be used to estimate the exciton binding energy in unscreened environments.

3:18PM D28.00005 Direct Measurement of Strain-induced Changes in Carbon Nanotube Bandstructure , MINGYUAN HUANG, Columbia University, YANG WU, BHUPESH CHANDRA, YUYAO SHAN, TONY HEINZ, JAMES HONE, Columbia University — The transition energies of single-walled carbon nanotubes under uniaxial strain were measured by Rayleigh scattering spectroscopy. The transitions display significant strain-induced shifts, as predicted by theory. In semiconducting tubes, successive transitions shift in opposite directions. In chiral metals, the split peaks merge with strain. We also observe small, but measurable shifts in the transitions of armchair tubes. The behavior is qualitatively consistent with theoretical predictions based on the trigonal warping effect in nanotube bandstructure.

3:30PM D28.00006 Raman Spectroscopy of Axially Strain Carbon Nanotubes , RAJAY KUMAR, STEPHEN CRONIN, University of Southern California — We investigate resonant Raman scattering of carbon nanotube bundles on an elastomer substrate under axial strains as high as 15%. Over the applied strain range, the G band Raman frequency decreases for both metallic and semiconducting nanotubes. The G` band Raman spectra, however, respond differently to strain for metallic and semiconducting nanotubes, giving insight into the nature of the broad metallic G band lineshape. The G` band frequency downshifts with applied strain for semiconducting nanotubes, while the G` band frequency increases with strain for metallic nanotubes. The G` band linewidth of metallic nanotubes also becomes narrower with strain, making it appear more semiconductor-like. Surprisingly, this metal to semiconductor transition is not reversible with strain, which indicates that nanotube-nanotube coupling plays a role in the observed broad G` band lineshape of metallic nanotubes.

3:42PM D28.00007 Optical Spectroscopy of Individual Carbon Nanotubes , FENG WANG, UC Berkeley — Single-walled carbon nanotubes (SWNTs) constitute a family of more than 100 one-dimensional structures. With properties varying significantly as a function of their precise atomic structure and environment, SWNTs provide a rich material system to study 1-dimensional physics. To unravel the wealth of different behavior in the SWNTs, which range from metallic to semiconducting, it is generally desirable, and often essential, to probe them individually. In this talk, I will describe the development and application of three techniques for optical spectroscopy of individual SWNTs: Rayleigh scattering, multiphonon-Raman scattering and absorption spectroscopy. We will illustrate the range of physical information attainable from these methods, including analysis of the excited electronic states of semiconducting and metallic nanotubes, nanotube-nanotube interactions and electron-phonon coupling. In addition to their separate use, these spectroscopies can also be fruitfully combined with one another and with other complementary non-optical, single nanotube characterization methods. The correlation of Rayleigh scattering with multi-phonon Raman measurements provides, for example, direct information on the resonance enhancement of electron-phonon interaction. On the other hand, application of Rayleigh scattering in conjunction with single nanotube electron diffraction has permitted us to obtain electronic spectra of SWNTs of independently determined structure. These measurements have permitted verification of the underlying theoretical trends used in previous assignments of nanotube optical spectra. Work done in collaboration with: D. Cho, W. Liu, B. Kessler, A. Zettl, Y. R. Shen (UC Berkeley and LBNL), J. Schuck (LBNL), T. Beetz, J. A. Misewich, L. Wu, Y. Zhu, M. Y. Sfeir (Brookhaven National Lab), and Y. Wu, L. Huang, J. Hone, S. O’Brien, L. E. Brus, and T. F. Heinz (Columbia University).

4:18PM D28.00008 Direct Measurement of the Quantum Yield of Isolated Single Walled Carbon Nanotubes , LISA CARLSON, TODD KRAUSS, University of Rochester — Owing to their unique optical properties, single walled carbon nanotubes (SWNTs) have received much recent attention. However, questions remain about whether the fluorescence quantum yield (QY) varies among SWNT samples. Using a confocal microscopy and digital imaging system, singlet SWNTs were doped in a nonpolar semicrystalline polymer (PS) matrix, dispersed with micelles in sodium cholate surfactant in D$_2$O; dilute mixtures of SWNTs and QDs were then spin cast onto quartz and their fluorescence intensities were directly compared. By accounting for differences in the absorption cross sections between the systems, the SWNT QY was determined to be $\sim$2%, nearly two orders of magnitude greater than the ensemble measurement. We will report on whether the measured QY represents an intrinsic nanotube property or if it depends upon other factors such as local environment, intertube interactions, and defects.
4:30PM D28.00009 Low Temperature Micro-photoluminescence and Raman Spectroscopy of Single-Walled Carbon Nanotubes. AJIT SRINIVASTAVA, ERIK HAROZ, YOICHI MURAKAMI, JUNICHIRO KONO, Rice University — We report micro-photoluminescence (PL) and resonance Raman spectroscopy studies performed on single-walled carbon nanotubes at low temperatures. At sufficiently low temperatures, where the thermal energy kT is smaller than the predicted dark-bright exciton splitting, PL is expected to be quenched as excitons populate only the dark ground state. However, we observe strong PL from single tubes with very sharp linewidths (∼ 1 meV for 1 nm diameter tubes) even at temperatures as low as 5 K. We will discuss the origin of this emission. We also study the PL linewidth as a function of temperature in order to provide insight into the PL line-broadening mechanisms. Resonance micro-Raman spectroscopy of single tubes was also performed at cryogenic temperatures, scanning the wavelength of the excitation laser beam around the E22 transition of the nanotubes, which revealed rich structure both in the vibrational spectrum and the excitation profile. The temperature dependence of various Raman features will be presented.

4:42PM D28.00010 Photoluminescence from inter-tube carrier migration in single-walled carbon nanotube bundles. O. N. TORRENS, D. E. MILKIE, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, M. ZHENG, DuPont Central Research and Development Experimental Station, Wilmington, DE 19880, J. M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — We detect new, dominant PL features from aqueous suspensions of single-walled carbon nanotubes (SWNTs) associated with energy transfer between semiconducting species in SWNT bundles. In these bundles, excitons are resonantly photoexcited at the E22 excitonic transition of populous, large bandgap SWNTs ((6,5), (7,5), and (8,3)). Excited excitons then efficiently migrate to smaller bandgap SWNTs ((7,6), (8,4), and (9,2)) and radiatively relax by emitting photons resonant with the E11 excitonic transition of these less common species. These energy transfer (ET) emission peaks demonstrate efficient exciton coupling between different SWNT species within bundles. Aqueous SWNT solutions with low levels of metallic SWNTs prevent quenching of bundle PL, and linear dichroism measurements of SWNT magnetic alignment detect bundle formation.[1] O. N. Torrens, D. E. Milkie, M. Zheng, J. M. Kikkawa, Nano Lett. (in press).

≤Supported by NSF DMR-0520020 and DMR-0094156.

4:54PM D28.00011 Unique Optical and Electrical Properties of Almost-Isolated Vertically Aligned Single-Walled Carbon Nanotubes. SHIGEO MARUYAMA, ERIK EINARSSON, MASAYUKI KADOWAKI, ZHENG YI ZHANG, Dept. Mech. Eng., The University of Tokyo — A new insight is gained on the structure of the vertically aligned single-wall carbon nanotubes (VA-SWNTs) generated by ACCVD technique. Our recent finding of the simple removal method using hot-water enabled us to transfer this film to various flat substrates. Transferring this film on TEM grid made it possible to directly observe the morphology of nanotubes from the top. To our surprise, the average number of nanotubes of a bundle is less than about 10. Electronic properties measured by EELS revealed that nanotubes are virtually electronically isolated. Then, the characteristic resonant Raman features are reconsidered. The high resolution Raman measurements show the sharp features for the RBM peak which have been assigned to cross-polarized resonance. The isolated and cross-polarized absorption resonance in Raman will be discussed based on the recent identification of the excitonic cross-polarized absorption through photoluminescence spectroscopy.

5:06PM D28.00012 Absolute potential of the Fermi level of single-walled carbon nanotubes via hydrogenase complex formation. TIMOTHY MCDONALD, DRAZENKA SVEDRUZIC, YONG-HYUN KIM, JEFFREY BLACKBURN, SHENGBAGI ZHANG, PAUL KING, MICHAEL HEBEN, National Renewable Energy Lab — The absolute potential of the Fermi level of nanotubes as a function of nanotube type is not presently understood, and is important for many nanotube applications and sorting strategies. Here, we study complexes of recombinant [FeFe] hydrogenases and single-walled carbon nanotubes. We find evidence that novel charge-transfer complexes are formed and are stable, which enables further study and application of this system. The hydrogenase functions as a hydrogen electrode sensitizing the nanotubes to the redox half-reaction for hydrogen. Thus the potential can be altered by changing the molecular hydrogen concentration, and this tunability is utilized to bleach various semiconducting nanotube transitions. By observing which are bleached and which remain emissive, we determine the alignment of the potential of the Fermi level of semiconducting single-walled carbon nanotubes. The experimentally determined Fermi level alignment is confirmed theoretically by the first-principles DFT-PBE method.[1] Supported by DOE Solar Photochemistry program, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences.

1Supported by DOE Solar Photochemistry program, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences.

5:18PM D28.00013 i—Carrageenan as a Matrix for Carbon Nanotube Spectroscopy. WILLIAM RICE, YOICHI MURAKAMI, JUNICHIRO KONO, ÉCE Dept. at Rice University — We have developed films of individualized single-walled carbon nanotubes (SWNTs) for spectroscopic studies using i—carrageenan, a polysaccharide macromolecule with a double helix structure, which is extruded from red seaweed. SWNTs produced by both the HiPco and CoMoCAT methods were separated using sodium cholate surfactants and ultracentrifugation. We found that for both HiPco and CoMoCAT tubes, the introduction of i—carrageenan did not significantly affect the interband optical absorption spectrum, indicating that separation was largely maintained. Further, we show that the optical density of the film is low in the mid-infrared (∼3.5 – 6 µm). This transparency is observed at temperatures as low as 4.2 K, making this film a good candidate for temperature-dependent spectroscopic studies of nanotubes. In addition, we confirmed that the polymer film transmits in the terahertz regime (.2 – .9 THz).

Monday, March 5, 2007 2:30PM - 5:30PM –
Session D39 FIAP DMP: Focus Session: Materials and Applications for Solar Energy II
Colorado Convention Center 502

2:30PM D39.00001 Intermediate- band solar cells: future prospects and challenges. ANTONIO MARTI, Instituto de Energia Solar - Universidad Politecnica de Madrid — The intermediate band solar cell is a novel type of solar cell with the potential of exceeding the limiting efficiency of single gap solar cells. Its principle of operation relies on the existence of a material characterized by an electronic band (intermediate band) located within the semiconductor bandgap. This intermediate band allows the absorption of two below-band gap energy photons to produce one electron-hole pair and is engineered to prevent introducing non-radiative recombination mechanisms in the cell. This basic principle of operation has been recently experimentally demonstrated in devices employing InAs/GaAs quantum dots. In this system, the intermediate band arises from the energy states associated to the confinement of the electrons in the dots. The challenges for the future are: a) to produce devices in which the intermediate band effect is enhanced, b) to identify and synthesize other intermediate band material systems, maybe different from the ones based on quantum dots and c) to produce high efficiency devices that allow the production of photovoltaic electricity at competitive costs.

1FULLSPECTRUM-European Commission (SES6-CT-2003-502620); Consolider-GenesisFV(CSD2006-00004); NUMANCIA (S-0505/ENE/000310)
3:06PM D39.00002 Materials characterization and optimization in silicon heterojunction solar cells using spectroscopic ellipsometry, DEAN LEVI, EUGENE IVANICZKO, QI WANG, HOWARD BRANZ, National Renewable Energy Laboratory. — Silicon heterojunction solar cells (SHJ) utilize very thin (3-5 nm) layers of amorphous silicon deposited on the surface of crystalline silicon to produce very high efficiency solar cells with low temperature processing. Our research team has used hot wire chemical vapor deposition (HWCDV) to fabricate SHJ solar cells on p-type FZ silicon with efficiencies as high as 18.2%. The best cells are deposited on textured (100) silicon substrates where the texturing process creates pyramidal facets with (111) crystal faces. One of the key factors in maximizing the efficiency of our SHJ devices is the process of optimizing the material properties of the amorphous silicon (a-Si) layers used to create the junction and back contact in these cells. Such optimization is technically challenging because of the difficulty in measuring the properties of extremely thin layers. This difficulty is compounded by the fact that the properties of such amorphous layers are substrate- and thickness-dependent. We report in this study how the substrate temperature and substrate orientation affect the structural, optical, and electronic properties of the a-Si layers used in our SHJ devices, and how these properties affect the final device performance.

3:18PM D39.00003 Characterization of Grain Boundaries in Polycrystalline Photovoltaic Devices using Near-Field Scanning Optical Microscopy, J.M. YARBROUGH, I.C. SCHICK, V. KAYDANOV, T.R. OHNO, R.T. COLLINS, Colorado School of Mines. — Polycrystalline thin film PV devices have the potential to reduce the cost per watt for commercial photovoltaic, but, their lower efficiency compared to their counter parts and lack of stability have prevented their widespread adoption. There is a need for a more fundamental understanding of these PV devices. A near-field scanning optical microscope (NSOM) has been built to optically and electrically characterize polycrystalline thin film PV devices. The NSOM is presently being used in air and at room temperature to perform spatially resolved photocurrent measurements using a broad range of visible excitation wavelengths on planar PV devices. Results from the front side illuminated planar CdTe devices show between a 5 and 10% increase in the generated photocurrent between the grains supporting the idea of charge separation at the grain boundary. Unlike previous studies, these photocurrent measurements have been decoupled from the topographical cross talk typically common to NSOM measurements. The authors gratefully acknowledge support from the National Science Foundation under Grant No. DMR-0103945 and samples provided by the University of Toledo.

3:30PM D39.00004 Theory of photo-conversion in polycrystalline silicon, A.I. SHKREBTII, University of Ontario Institute of Technology, Oshawa, Canada, A.V. SACHENKO, A.P. GORBAN, V.P. KOSTYLIOV, I.O. SOKOLOVSKY, V. Lashkarev Institute of Semiconductor Physics, Kiev, Ukraine, A. KAZAKEVITCH, University of Ontario Institute of Technology, Oshawa, Canada. — We developed a three-dimensional analytical formalism of photo-conversion in polycrystalline silicon based solar cells. Polycrystalline Si was modeled by representing the grains as parallelepipeds or cylinders, considering spatial dependence of generation and recombination of electron-hole pairs both in the bulk and at the grain boundaries. We calculated spectral dependence of the short circuit current and open circuit voltage over the grain. The recombination of the photo carriers at the grain boundary was described by introducing the effective diffusion length, responsible for the attenuation of excess electron–hole pairs. The recombination dependence on the bulk diffusion length, grain size and effective recombination velocity at the boundaries were derived and discussed. The short circuit current, open circuit voltage and photo-conversion efficiency in polycrystalline Si are in good agreement with the experimental data available. The research was supported by the Centre for Materials and Manufacturing/Ontario Centres of Excellence (OCE/CMM) “Sonus/PV Photovoltaic Highway Traffic Noise Barrier” project.

3:42PM D39.00005 Photovoltaic applications of hydrogenated amorphous silicon thin films grown by the Saddle Field Glow Discharge Method, F. GASPARI, A.I. SHKREBTII, University of Ontario Institute of Technology (UOIT), Oshawa, Canada, A. KAZAKEVITCH, UOIT, A.V. SACHENKO, I.O. SOKOLOVSKY, V. Lashkarev Institute of Semiconductor Physics NAS, Ukraine, N. KHERANI, Electrical & Computer Engineering, University of Toronto, Canada, T. TEATRO, J. PERZ, UOIT. — Thin film hydrogenated amorphous silicon (a-Si:H) is widely used for photovoltaic solar cells. We present a combined theoretical and experimental study of the thin a-Si:H films for efficient and inexpensive solar cells, grown by the Saddle Field Glow Discharge Method. The type of solar cell studied is glass/SnO$_2$/p-i-n Si:H/Al. We investigated the mechanism of hydrogen diffusion inside the film, its relation to the bonding within the amorphous silicon network. Hydrogen diffusion in a-Si:H was modeled using first-principles finite temperature molecular dynamics. Optimization of the solar cells was performed based on the experimental diffusion coefficients, carrier mobilities, parameters of the p-i-n structures, and electron band structure (defect distribution inside the gap). An analytical model to optimize photo-conversion efficiency of a-Si:H based solar cells with contact grid has been developed. The research was supported by the Centre for Materials and Manufacturing/Ontario Centres of Excellence (OCE/CMM) “Sonus/PV Photovoltaic Highway Traffic Noise Barrier” project.

3:54PM D39.00006 Simple method to examine the work function of transparent conducting oxide for traditional and organic based photovoltaics, JOSEPH BERRY, MATTHEW REESE, JOHN PERKINS, DAVID GINLEY, National Renewable Energy Laboratory, NATIONAL CENTER FOR PHOTOVOLTAICS — Transparent conducting oxides (TCOs) are key components in both traditional and organic based optoelectronic devices. In photovoltaic applications in which TCOs are employed as transparent electrical contacts, the matching of the TCO work function to that of the active material is critical to device performance. We report the adaptation of a commercial electrostatic voltmeter to measure the work function of In$_2$O$_3$ and other TCO materials relevant to photovoltaics. The applicability of this technique to high-throughput combinatorial studies of compositionally graded TCO libraries will be presented. We will also examine correlations between the observed work function and other material properties in these TCO libraries. The relationship between device performance and the measured work function will also be assessed.

4:06PM D39.00007 Combinatorial Development of Amorphous Mixed Metal Oxide Transparent Conductors, J.D. PERKINS, M.F.A.M. VAN HEST, National Renewable Energy Lab, M.I. BERTONI, Northwestern Univ., C.W. TEPLIN, J.J. BERRY, J.L. ALLEMAN, M.S. DABNEY, I.M. GEDVILAS, B.M. KEYES, B. TO, National Renewable Energy Lab, A. LEENHEER, M.P. TAYLOR, DENNIS READEY, R. O’HAYRE, R. O’HAYRE, Colorado School of Mines, D.S. GINLEY, National Renewable Energy Lab — We are using combinatorial approaches to optimize both amorphous In$_2$O$_3$ (a-IZO) and amorphous Zn$_5$Sn$_2$O$_8$ (a-ZTO) transparent conductors for photovoltaic applications. Compositionally-graded combinatorial samples (“libraries”) are deposited by co-sputtering onto 2”x2” glass substrates at temperatures ranging from room-temperature to 500 °C. Three to five libraries are generally required to cover the full composition range for a binary tie-line, such as from In$_2$O$_3$ to ZnO. For IZO, we have found that IZO films deposited in Ar at 100 °C are amorphous for films with 65 to 85 cation% In, with a maximum conductivity of 3000 S/cm at 80 cation% In and an RMS roughness of 0.4 nm. Subsequent sequential annealing experiments in both Ar and air show that a-IZO films are structurally, electrically and optically quite robust for anneals up to 500 or 600 °C. For a-ZTO, the best conductivity obtained to date for an amorphous ZTO film is 200 S/cm for films grown at 400 °C with 35 cation% Zn.
4:18PM D39.00008 Optimization of amorphous In-Zn-O (IZO) transparent conductor sputtered at ambient temperature, ANDREW LEENEHER, Colorado School of Mines, JOHN PERKINS, National Renewable Energy Laboratory, ANDREW CAVENDOR, Colorado School of Mines, MATTHEW TAYLOR, MAIKEL VAN HEST, DAVID GINLEY, National Renewable Energy Laboratory — Amorphous indium zinc oxide (IZO) is an n-type transparent conducting oxide (TCO) that offers high electrical conductivity, visible-spectrum transparency, smoothness and ease of deposition, all properties of interest for photovoltaic and optoelectronic applications. Previous work has shown that magnetron-sputtered IZO is amorphous over the metals-only composition range ~55 to 85 atomic % indium. In this work, five different single-composition targets spanning the amorphous range were used to sputter thin films at ambient temperature with varying oxygen content in the sputter gas. In addition, highly resistive films were deposited to make field-effect thin-film transistors. The resistivity, carrier concentration, and hall mobility, as well as the optical transmission and reflection for λ=300-900 nm light were measured for each film. The conductivity was tunable from ~2.5 x 10^4 S/cm to ~10^{-1} S/cm depending on the amount of oxygen present. Generally, increasing the oxygen or lowering the indium content lowers the carrier concentration, while increasing the indium content increases the electron mobility. For thin-film transistors, a low carrier concentration but high mobility is desired.

4:30PM D39.00009 Transparent Conducting ZnO Thin Films Doped with Al and Mo, JOEL DUENOW, Department of Chemical and Environmental Engineering, Colorado School of Mines, TIMOTHY GESSERT, National Renewable Energy Laboratory, DAVID WOOD, Colorado School of Mines, DAVID YOUNG, TIMOTHY COUTTS, National Renewable Energy Laboratory — Transparent conducting oxide (TCO) thin films are a vital part of photovoltaic cells, flat-panel displays, and electrochromic windows. ZnO-based TCOs, due to the relative abundance of Zn, may reduce production costs compared to those of the prevalent TCO In_{2-x}O_x-Sn (ITO). Undoped ZnO, ZnO:Al (0.5, 1, and 2 wt.% Al_{2}O_{3}), and ZnO:Mo (2 wt.% Mo) films were deposited by RF magnetron sputtering. Optimal deposition temperature was found to be 200°C. Controlled incorporation of H_2 in the Ar sputtering ambient increased mobility of undoped ZnO significantly to 48 cm^2V^{-1}s^{-1}. H_2 also appears to catalyze ionization of dopants. This enabled lightly doped ZnO:Al to provide comparable conductivity to the standard 2 wt.%-doped ZnO:Al while demonstrating reduced infrared absorption. Mo was found to be an n-type dopant of ZnO, though material properties did not match those of ZnO:Al. Scattering mechanisms were investigated using temperature-dependent Hall measurements and the method of four coefficients. This abstract is subject to government rights.

4:42PM D39.00010 A theoretical study on native point defects and dopants in cuprous oxide, WEICHAO WANG, DANGXIN WU, QIMING ZHANG, Department of Physics, University of Texas at Arlington, MENG TAO, Department of EE, University of Texas at Arlington — We have performed a first-principle study on the electronic structures, atomic configurations, and formation energies of native point defects in cuprous oxide, i.e. vacancies (V_{Cu}, V_{O}), interstitials (I_{Cu}, I_{O}), and antisite defects (Cu_{O}, O_{Cu}) by using Density Function Theory based VASP package with PAW potentials. We have carefully studied the formation of native point defects under different chemical environments and Fermi level positions. We have also calculated the electronic structures of dopants such as F, Cl, N, Ca and Mg in the cuprous oxide crystal. Their formation at different chemical environments and Fermi level positions will be presented as well.

4:54PM D39.00011 Thin film preparation of the p-type transparent semiconductor Cu_3TaS_4, PAUL NEWHOUSE, Department of Physics, Oregon State University, PETER HERSH, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, CHEOL-HEE PARK, Department of Chemistry, Oregon State University, PAUL NEWHOUSE, Department of Physics, Oregon State University, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, JANET TATE, Department of Physics, Oregon State University — Thin films of a new wide band gap p-type semiconductor Cu_3TaS_4 (CTS) are prepared by PLD deposition of Cu and Ta metal multilayers and subsequent ex-situ rapid thermal processing in a sulfur environment. X-ray diffraction confirmed the presence of single phase CTS. 275 nm thick CTS films on fused SiO_2 substrates show reflection-corrected transmission >70% over the range 400-700 nm, with an optical band gap near 2.8 eV. The electrical resistivity of undoped CTS thin films is ~ 5 Ohm cm. These properties indicate that CTS thin films may find application in transparent electronics.

5:06PM D39.00012 Properties of a potential transparent p-type semiconductor Cu_3TaQ_1 (Q = S or Se), PETER HERSH, Department of Chemistry, Oregon State University, PAUL NEWHOUSE, Department of Physics, Oregon State University, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, JANET TATE, Department of Physics, Oregon State University — Physical, optical and electrical properties of powder samples of the Cu_3TaQ_1 (Q = S or Se) series are investigated to determine the potential as a transparent semiconductor. The series crystallizes in a P-43m sulfanite structure. The sulfide has a lattice parameter of a = 5.6535(7) Å and the selenide has a lattice parameter of a = 5.6306(4) Å. The optical band gaps are 2.77 eV for Cu_3TaS_4 and 2.36 eV for Cu_3TaSe_4. Seebeck coefficients of +27 µV/K for Cu_3TaS_4 and +24µV/K for Cu_3TaSe_4 confirm that both materials are p-type. FLAPW band structure calculations indicate that the band gap is indirect.

5:18PM D39.00013 Transparent conductive BaCuTeF thin films by pulsed laser deposition, ROBERT KYKYNESHI, DAVID MCINTYRE, JANET TATE, Department of Physics, Oregon State University, Corvallis, OR 97331, CHEOL-HEE PARK, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR 97331, TRANSPARENT CONDUCTORS TEAM — Transparent p-type carrier conductive BaCuTeF thin films are reported. Undoped BaCuTeF films obtained in-situ by pulsed laser deposition in UHV exhibit maximum conductivities of 50-55 S/cm on fused silica substrates. The polycrystalline films deposited at various temperatures up to 600°C are single phase with optical band gap of about 3 eV and 70% average transparency in the visible and near-IR optical ranges. BaCuTeF films deposited on single crystal MgO substrates are highly oriented.

1 Supported by the National Science Foundation

5:18PM D39.00013 Transparent conductive BaCuTeF thin films by pulsed laser deposition, ROBERT KYKYNESHI, DAVID MCINTYRE, JANET TATE, Department of Physics, Oregon State University, Corvallis, OR 97331, CHEOL-HEE PARK, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR 97331, TRANSPARENT CONDUCTORS TEAM — Transparent p-type carrier conductive BaCuTeF thin films are reported. Undoped BaCuTeF films obtained in-situ by pulsed laser deposition in UHV exhibit maximum conductivities of 50-55 S/cm on fused silica substrates. The polycrystalline films deposited at various temperatures up to 600°C are single phase with optical band gap of about 3 eV and 70% average transparency in the visible and near-IR optical ranges. BaCuTeF films deposited on single crystal MgO substrates are highly oriented.

1 Supported by the National Science Foundation

5:18PM D39.00013 Transparent conductive BaCuTeF thin films by pulsed laser deposition, ROBERT KYKYNESHI, DAVID MCINTYRE, JANET TATE, Department of Physics, Oregon State University, Corvallis, OR 97331, CHEOL-HEE PARK, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR 97331, TRANSPARENT CONDUCTORS TEAM — Transparent p-type carrier conductive BaCuTeF thin films are reported. Undoped BaCuTeF films obtained in-situ by pulsed laser deposition in UHV exhibit maximum conductivities of 50-55 S/cm on fused silica substrates. The polycrystalline films deposited at various temperatures up to 600°C are single phase with optical band gap of about 3 eV and 70% average transparency in the visible and near-IR optical ranges. BaCuTeF films deposited on single crystal MgO substrates are highly oriented.

1 Supported by the National Science Foundation

5:18PM D39.00013 Transparent conductive BaCuTeF thin films by pulsed laser deposition, ROBERT KYKYNESHI, DAVID MCINTYRE, JANET TATE, Department of Physics, Oregon State University, Corvallis, OR 97331, CHEOL-HEE PARK, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR 97331, TRANSPARENT CONDUCTORS TEAM — Transparent p-type carrier conductive BaCuTeF thin films are reported. Undoped BaCuTeF films obtained in-situ by pulsed laser deposition in UHV exhibit maximum conductivities of 50-55 S/cm on fused silica substrates. The polycrystalline films deposited at various temperatures up to 600°C are single phase with optical band gap of about 3 eV and 70% average transparency in the visible and near-IR optical ranges. BaCuTeF films deposited on single crystal MgO substrates are highly oriented.

1 Supported by the National Science Foundation

5:18PM D39.00013 Transparent conductive BaCuTeF thin films by pulsed laser deposition, ROBERT KYKYNESHI, DAVID MCINTYRE, JANET TATE, Department of Physics, Oregon State University, Corvallis, OR 97331, CHEOL-HEE PARK, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR 97331, TRANSPARENT CONDUCTORS TEAM — Transparent p-type carrier conductive BaCuTeF thin films are reported. Undoped BaCuTeF films obtained in-situ by pulsed laser deposition in UHV exhibit maximum conductivities of 50-55 S/cm on fused silica substrates. The polycrystalline films deposited at various temperatures up to 600°C are single phase with optical band gap of about 3 eV and 70% average transparency in the visible and near-IR optical ranges. BaCuTeF films deposited on single crystal MgO substrates are highly oriented.

1 Supported by the National Science Foundation
2:30PM D44.00001 Optical control and determination of charge in self-assembled quantum dots, M. KORKUSINSKI, P. HAWRYLAK, IMS NRC, Ottawa, Canada, A. BABINSKI, Warsaw University, Poland, M. POTEMSKI, GHMFL, CNRS Grenoble, France, S. RAYMOND, J. LAPONTE, Z. WASILEWSKI, IMS NRC, Ottawa, Canada — We present a theory and experiment allowing for optical control of charge in a single InAs/GaAs quantum dot (QD) in magnetic fields up to 23 T [1]. The charge is controlled by excitation energy and power and is determined by comparing the experimental PL spectra of the QD to the ones calculated for N electrons and one hole using the parabolic confinement and the CI technique for many-carrier states. The number N is determined from the characteristic features in PL [2]. For N=4 electrons in low fields the degenerate p shell is half-filled and the system is in a triplet state. At larger fields the degeneracy is removed and a triplet-singlet transition occurs. This transition is seen as a discontinuity in the magnetic-field dependence of PL lines. In even higher fields, electrons increase their polarization through spin-flip transitions, which also leads to discontinuities of the PL spectra. Also, as the magnetic moment of electrons increases, the electron-hole exchange leads to the appearance of multiple PL lines. [1] A. Babinski et al, Physica E 26, 190 (2005) [2] A. Wojs and P. Hawrylak, Phys. Rev. B 55, 13066 (1997)

2:42PM D44.00002 Spin effects in coupled quantum dots under ac electric fields, LILIA MEZAMONTES, Instituto de Física BUAP, Apdo. Postal J-48, Puebla, Pue., 72570 Mexico, AREZKY H. HERNANDEZ, Instituto de Física UNAM, Mexico, SERGIO E. ULLOA, CMSS & NQPI Ohio University, Clipp Labs, Athens, Ohio 45701 — Spin control has recently attracted attention for applications in spin-based devices. Different effects and applied fields have been suggested to accomplish the goal. We explore the time evolution of electronic spin in coupled quantum dots under harmonic electric fields. Using the Floquet formalism, we obtain the time dependent wave function in terms of the Floquet states and the quasi-energy spectrum for a single electron in double InSb dots. The spatial part of the wave function includes the VIA and BIA spin-orbit effects. The spectral force is analyzed at anti-crossings of the quasi-energy bands as a function of the field strength. The resulting dynamical symmetries and the way they reflect in the time evolution of the spin clouds will be discussed.

1Partially supported by Condensed Matter and Surface Science Program & Nanoscale and Quantum Phenomena Institute, OU.

2On sabbatical leave at Ohio University.

2:54PM D44.00003 Qubit identification and entanglement in tunneling and Förster coupled quantum dots, JUAN E. ROLON, SERGIO E. ULLOA, Ohio University — We investigate the possibility of qubit coherent manipulation using the multi-excitonic optical spectrum features of a quantum dot molecule (QDM), a system of two vertically coupled InAs/GaAs self-assembled quantum dots. The spectrum is modeled using a Hamiltonian that incorporates coupling dependence on several experimental parameters, such as gate voltage, optical excitation intensity and its detuning. We use realistic structure parameters to describe the important coupling constants, including electron and hole tunneling, and Coulomb correlations that depend on the QDM strain field, and interdot distance [1]. We also incorporate the role of the Förster-Dexter resonant energy transfer processes, as well as, exciton oscillator strengths extracted from available PL spectroscopy data. The dynamics given by the time evolution of the density matrix and the qubit-quantuming contest interaction is monitored by calculations of the entanglement of formation [2] for the suitable excitonic molecular states. We discuss how to optimize Rabi flops and entanglement via gate-controlled adiabatic passage through a level anticrossing [3]. [1] G. Bester, A. Zunger, PRB 71 075325 (2005) [2] W.K. Wootters, PRL 80(10) 2245 (1998) [3] K. Bergmann, Rev. Mod. Phys. 70(3) (1998)

3:06PM D44.00004 Spin Interactions in Optically Excited Quantum Dot Molecules, MICHAEL SCHEIBNER, Naval Research Laboratory Washington DC 20375 USA — Recently we have demonstrated controlled interaction between QDs [1] — a key requirement for the use of QDs as basic building blocks in novel information processing technologies, as e.g. in quantum computation or spintronics. Here we delineate for the first time the origin of the exchange coupling between spins [2] in optically excited QD molecules, and we trace its atomic to molecular evolution. We have performed photoluminescence spectroscopy on single InAs/GaAs QDMs. The QD molecules were formed by the subsequent growth of we delineate for the first time the origin of the exchange coupling between spins in optically excited QD molecules, and we trace its atomic to molecular evolution. We have performed photoluminescence spectroscopy on single InAs/GaAs QDMs. The QD molecules were formed by the subsequent growth of single-particle states. The interplay between tunneling, electron-electron, hole-hole and electron-hole exchange interactions splits the states with different spin-projections. The model explains a rich diversity of spectral line patterns in photoluminescence spectra observed in recent experiments. [1] E.A.Stinaff et al., Science 311, 636 (2006). [2] I.V. Ponomarev et al., Phys. Stat. Sol. (b), 243, 3869. (2006)

3:24PM D44.00005 Theory of Spin States in Coupled Quantum Dots, ILYA PONOMAREV, MATT DOTY, MICHAEL SCHEIBNER, ALLAN BRACKER, DAN GAMMON, TOM REINECKE, Naval Research Laboratory, Washington DC — The system of vertically coupled self-assembled quantum dots (CQDs) tuned by external electric field is a promising candidate as a basis for coherent optical spin manipulation in quantum information applications and spintronics [1]. We have developed a theoretical model that describes spin states of neutral and charged excitons in CQDs [2]. In this approach the electric field induced resonant tunneling of the electron and hole states occurs at different biases due to the inherent asymmetry of CQDs. The truncated many-body basis configurations for each molecule are constructed from antisymmetrized products of single-particle states. The interplay between tunneling, electron-electron, hole-hole and electron-hole exchange interactions splits the states with different spin-projections. The model explains a rich diversity of spectral line patterns in photoluminescence spectra observed in recent experiments. [1] E.A.Stinaff et al., Science 311, 636 (2006). [2] I.V. Ponomarev et al., Phys. Stat. Sol. (b), 243, 3869. (2006)

3:54PM D44.00006 Polarized stimulated emission from photonic molecule states in coupled microdisk lasers, X. LI, B.J. COOLEY, N. SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802. F.M. MENDOZA, R.C. MYERS, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara CA 93106 — Recent studies have demonstrated the engineering of spin coherence via photon-spin interactions in microdisk lasers. [S. Ghosh et al., Nature (Materials) 5, 261 (2006)], motivating the theoretical advancement of such measurements to understand the interplay between spin and photon coherence in microdisk lasers. In this approach the electric field induced resonant tunneling of the electron and hole states occurs at different biases due to the inherent asymmetry of coupled microdisks. The reduced many-body basis configurations for each molecule are constructed from antisymmetrized products of single-particle states. The interplay between tunneling, electron-electron, hole-hole and electron-hole exchange interactions splits the states with different spin-projections. The model explains a rich diversity of spectral line patterns in photoluminescence spectra observed in recent experiments. [1] E.A.Stinaff et al., Science 311, 636 (2006). [2] I.V. Ponomarev et al., Phys. Stat. Sol. (b), 243, 3869. (2006)

4:06PM D44.00007 ABSTRACT WITHDRAWN
4:18PM D44.00008 Spin Multiphoton Antiresonance at Finite Temperatures, CHRISTIAN HICKE, MARK DYKMAN, Michigan State University — Weakly anisotropic $S > 1$ spin systems display multiphoton antiresonance. It occurs when an Nth overtone of the radiation frequency coincides with the distance between the ground and the Nth excited energy level (divided by $\hbar$). The coherent response of the spin displays a sharp minimum or maximum as a function of frequency, depending on which state was initially occupied. We find the spectral shape of the response dips/peaks. We also study the stationary response for zero and finite temperatures. The response changes dramatically with increasing temperature, when excited states become occupied even in the absence of radiation. The change is due primarily to the increasing role of single-photon resonances between excited states, which occur at the same frequencies as multiphoton resonances. Single-photon resonances are broad, because the single-photon Rabi frequencies largely exceed the multi-photon ones. This allows us to separate different resonances and to study their spectral shape. We also study the change of the spectrum due to relaxational broadening of the peaks, with account taken of both decay and phase modulation.

4:30PM D44.00009 Nonlinear interlevel optical phenomena in quantum dots, VICTOR BONDARENKO, YANG ZHAO, WSU — Nonlinear interlevel optical phenomena caused by the electron-electron interaction in quantum dots are investigated theoretically within the semiclassical density matrix formalism. A special attention is paid to the intrinsic optical bistability. Obtained analytical relations and results of numerical simulation reveal role of driving characteristic parameters of quantum dot systems as well as of the incident radiation in the phenomena. Self-consistent treatment of the electron-electron interaction is shown to be of crucial importance. A proper microscopical treatment is shown to be needed for accurate description of the phenomena.

4:42PM D44.00010 Origin of second-harmonic generation of Si nanoinclusions in glass¹, E.J. ADLES, D.E. ASPNES, North Carolina State University — We applied our anisotropic bond model (ABM) to clarify the origin of the second-harmonic-generation (SHG) signals observed by Figliozzi et al.[1] for Si nanoinclusions in glass. The ABM describes nonlinear-optic (NLO) responses in terms of radiation from anisotropically and anharmonically bound bond charges, and differs from conventional force formulations by (1) incorporating anisotropy at the bond level and (2) describing observed NLO intensities as a coherent superposition of radiation from these charges accelerated by the driving field. It therefore provides specific information about the origins of NLO signals at the atomic level. Here, SHG signals from the glass and bulk of the Si inclusions are found to be essentially nonexistent, as expected,[2] in the former case as a result of cancellation of radiation fields of bonds oriented in random directions, and in the latter case due to dielectric screening. Our calculations show that SHG is dominated by gradient effects, specifically from the variation in field across the inclusion (spatial-dispersion and crossed-beam effects), consistent with experiment. The large interface field gradient contributes a weak signal from charge motion transverse to the bond direction. [1] P. Figliozzi et al. Phys Rev Lett 94 (2005). [2] V. L. Brudny et al. Phys Rev B 62 (2000).

¹Work supported by the Office of Naval Research.

4:54PM D44.00011 Rabi Coupling Between IR-active Phonon and Cavity-resonant Electromagnetic Modes¹, GAVIN K. BRENNEN, Institute for Quantum Optics and Information of the Austrian Academy of Sciences, H.M. LAWLER, University of Washington, SANJIV SHRESTA, NIST, J.N. BYRD, University of Washington — We predict an approximately 200 micron Rabi coupling between a cavity-resonant electromagnetic mode and the infrared-active phonon of an enclosed GaAs sample. This prediction follows from our quantized description of the electromagnetic field, the phonon field, and their interaction. We believe the predictions to be supported by recent observations of geometry-enhanced terahertz emission, and boundary-condition dependent phonon-polariton spectra in pump-probe optical studies.

¹This work was supported by the NRC and the ONR through the Naval Research Laboratory. J.N. Byrd was supported by the NSF REU program.

5:06PM D44.00012 Electron-Photon interaction associated Uncertainty Relation based Tunneling in a Parallel Double Quantum Dot System, KAO-CHIN LIN, Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan, DER-SAN CHIU COLLABORATION — A new mechanism of electron-photon interaction in a parallel double quantum dot (DQD) system is studied. The electron is allowed to tunnel between dots due to the electron-photon interaction. When the electron in quantum dot m (QDm) transits to the adjoining QDm(m,m1,2 and mm), it is allowed to tunnel into leadm, which is connected to QDm, via energy-time uncertainty relation in a very short time interval. Like the Kondo resonant peak in Anderson model, the new mechanism of the electron-photon interaction exhibits peaks which depends logarithmically on temperature. The character temperature obtained is found to be higher than the Kondo temperature in some situations. Unlike the Kondo effect, the quantum mechanical tunneling associated the electron-photon interaction is not always on resonance.

Tuesday, March 6, 2007 8:00AM - 11:00AM —
Session H4 DCOMP DCMP DMP: Recent Advances in quantum Monte Carlo Simulations
Colorado Convention Center Korbel 2B-3B

8:00AM H4.00001 Recent advances in auxiliary-field methods — simulations in lattice models and real materials¹, SHIWEI ZHANG, College of William and Mary — We have developed an auxiliary-field (AF) quantum Monte Carlo (QMC) method for many-body simulations. The method takes the form of a linear superposition of independent-particle calculations in fluctuating external fields. "Entanglement" of the different field configurations leads to random walks in Slater determinant space. We formulate an approximate constraint on the random walk paths to control the sign/phase problem, which has shown to be very accurate even with simple mean-field solutions as the constraining trial wave function. The same method can be applied to both simplified lattice models and real materials. For realistic electronic Hamiltonians, each random walk stream resembles a density-functional theory (DFT) calculation in random local fields. Thus, the AF QMC method can directly import existing technology from standard electronic structure methods into a many-body QMC framework. We have demonstrated this method with calculations in close to 100 systems, including Si solid, first- and second-row molecular systems, molecules of heavier post-d elements, transition-metal systems, and ultra-cold atomic gases. In these we have operated largely in an automated mode, inputting the DFT or Hartree-Fock solutions as trial wave functions. The AF QMC results showed consistently good agreement with near-exact quantum chemistry results and/or experiment. I will also discuss additional algorithmic advances which can further improve the method in strongly correlated systems.

Supported by ARO, NSF, ONR, and DOE-cmsn.

¹In collaboration with W. A. Al-Saidi, Henry Krakauer, and Wirawan Purwanto
8:36AM H4.00002 Lattice regularized diffusion Monte Carlo method, MICHELE CASULA, Department of Physics, University of Illinois, Urbana-Champaign — We introduce a lattice regularization scheme for quantum Monte Carlo calculations of realistic electronic systems[1]. Our method is based on the discretization of a projection operator (Green’s function), constructed upon an effective regularized Hamiltonian[2]. In particular, its Laplacian is discretized with two incommensurate mesh sizes, \(a\) and \(a'\), where \(a'/a\) is a fixed irrational number, and the regularized Hamiltonian goes to the continuous limit for \(a \to 0\). The use of the double mesh improves significantly the convergence to the \(a \to 0\) limit, and allows one to take into account efficiently the different length scales in the system. Another advantage of this framework is the possibility to include non-local potentials in a consistent variational scheme, substantially improving both the accuracy and the computational stability upon previous non-variational diffusion Monte Carlo approaches. However, we have recently shown[3] that also the standard diffusion Monte Carlo algorithm can be made stable and variational even in the presence of non-local pseudopotentials, by including a non-local discrete process in the diffusion operator. This work can open the route for even more reliable and accurate electronic ground state calculations using diffusion Monte Carlo methods.

References:

9:12AM H4.00003 Pfaffian wave functions and topology of fermion nodes, LUBOS MITAS, North Carolina State University — Pfaffian is defined as a signed sum of all pair partitions of even number of elements and it can be viewed as a nontrivial generalization of determinant. Pfaffian enables to define the simplest possible antisymmetric wave function based on pair spinorbital(s) and therefore represents a pairing generalization of the Slater determinant of one-particle orbitals. Pfaffians actually accomodate several types of pairing wave functions, for example, one special case is the Bardeen-Cooper-Schrieffer wave function. Using this platform we propose pfaffian wave functions with simultaneous pairings both in singlet and triplet channels and we benchmark their performance in fixed-node quantum Monte Carlo. We implement Gaussian elimination-like algorithm which enables to calculate pfaffians with efficiency similar to calculation of determinants. For a testing set of first row atoms and molecules we show that single pfaffians provide correlation energies systematically at the level of about 95%. Linear combinations of small number of pfaffians recover another fraction of the missing correlation energy comparable to significantly larger determinantal expansions. In addition, we show that pfaffians possess an important property of fermionic wave functions, namely, the minimal number of two nodal domains defined by fermion nodes. This is related to the proof that under rather general conditions closed-shell ground states of fermionic systems in \(d \geq 1\) have two nodal domains for arbitrary system size. The explicit proofs cover a number of paradigmatic models such as fermions on a sphere surface, in a periodic box, atomic states, etc, and we discuss the implications of this on efficient construction of wave functions and on several types of many-body effects. Supported by NSF and done in collaboration with M. Bajdich, L.K. Wagner, G. Drobný, and K.E. Schmidt. Refs: L. Mitas, PRL 96, 240402 (2006); L. Mitas, cond-mat/0605550; M. Bajdich et al, PRL 96, 130201 (2006); cond-mat/0610850.

9:48AM H4.00004 QMC simulations using backflow correlated wave functions, RICHARD NEEDS, University of Cambridge — An inhomogeneous backflow transformation for many-particle wave functions is presented and applied to electrons in atoms, molecules, and solids. Backflow transformations are compact parametrizations, by which we mean that the number of parameters required to retrieve a given fraction of the correlation energy increases only slowly with system size. We report variational and diffusion quantum Monte Carlo (VMC and DMC) energies for a number of systems and study the computational cost of using backflow wave functions. Backflow transformations alter the nodal surface of the wave function and can therefore be used to reduce the fixed-node error in DMC calculations. Applications to the homogeneous electron gas, the all-electron lithium atom and dimer, and carbon atom and dimer, and pseudopotential calculations for the carbon atom and dimer and carbon diamond are presented. When the initial nodal surface is reasonably accurate, backflow appears to do an excellent job in improving the VMC energy and correcting the remaining errors in the nodal surface. When the initial nodal surface is poor, however, backflow is apparently incapable of making the gross changes to the nodal surface required to correct the flaws, although it still normally lowers both the VMC and DMC energies significantly. Overall, we find that inhomogeneous backflow transformations can provide a substantial increase in the amount of correlation energy retrieved within VMC and DMC calculations. This approach is of considerable generality as it is successful in metals and in insulators, and in large and small systems. Backflow transformations can readily be used with pairing wave functions, and this approach could yield significant improvements when a wave function consisting of a single determinant of one-particle orbitals is a poor starting point.

10:24AM H4.00005 Resonating Valence Bond wavefunctions for electronic simulations, SANDRO SORELLA, Democritos National Simulation Centre and SISSA — We discuss several progress for the simulation of strongly correlated electrons, based on an efficient implementation of the Resonating Valence Bond (RVB) theory with Quantum Monte Carlo (QMC). Due to very important advances[1] in the energy optimization of strongly correlated variational wave functions, it is now possible to optimize several variational parameters with remarkable efficiency even within a stochastic approach such as QMC. In this way it is possible to describe very accurately the electronic correlation by a first principle many-body wave function, that can be extended to fairly large electronic systems. Indeed a remarkable improvement of the Hartree-Fock theory is provided by the so called RVB wave function introduced by P.W. Anderson in the context of High-Tc superconductivity[2]. For instance, by means of this paradigm, it has been possible to perform a realistic and accurate simulation of the benzene dimer, where we have found that the RVB correlation of the benzene ring plays a crucial role in the dimer bonding[3,4]. Finally we consider the still controversial low-temperature and high-pressure phase diagram of Hydrogen by using the same RVB wavefunction. We use a novel second order Langevin dynamics by introducing a consistent friction tensor, allowing to remain in thermal equilibrium even with very noisy forces, namely determined by QMC with very short runs. This allows us to simulate finite temperature systems \((\simeq 100 \, \text{K})\) with very high efficiency, while the variational parameters are consistently optimized during the ionic dynamics.

References:

1supported by COFIN 2005 and CNR
8:00AM H8.00001 Large anisotropic normal-state magnetoresistance in clean MgB$_2$ thin films$^1$. QI LI, Penn State University — MgB$_2$ is arguably the first material which shows clear multiband superconductivity and two energy gaps. The interplay between the interband and intraband scattering as well as electron-phonon coupling has manifested in many physical properties. In this talk, I will review the magnetoresistance measurements of the normal state of MgB$_2$. We have shown large normal-state magnetoresistance with temperature-dependent anisotropy in very clean epitaxial MgB$_2$ thin films (residual resistivity much smaller than 1 $\mu\Omega$cm) grown by hybrid physical-chemical vapor deposition.$^1$ The magnetoresistance shows a complex dependence on the orientation of the applied magnetic field, with a maximum magnetoresistance (MR 136%) observed at the field $H$ parallel to $ab$ plane at low temperature. However, the angular dependence changes dramatically as the temperature is increased, and at high temperatures ($T > 100$ K), the magnetoresistance maximum changes to the $H$ perpendicular to $ab$ direction. We attribute the large magnetoresistance and the evolution of its angular dependence with temperature to the multiple bands with different Fermi surface topology in MgB$_2$ and the relative scattering rates of the $\sigma$ and $\pi$ bands, which vary with temperature due to stronger electron-phonon coupling for the sigma bands. The change of anisotropy with disorder has also been reported in neutron irradiated MgB$_2$ thin films.


$^1$Work is supported by NSF.

8:36AM H8.00002 Tunneling study of two-band superconductivity in MgB$_2$$^{1,2}$. KE CHEN, CHENGGANG ZHUANG$^2$, YI CUI, QI LI, XIAOXING XI$^3$, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania, USA; ZI-KUI LIU, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, USA — Thin film Pb/barrier/MgB$_2$ sandwich-type tunnel junctions have been fabricated. The MgB$_2$ films were epitaxially grown on (211) MgO substrates with c-axis tilted by 19.5 degrees with respect to the substrate normal by hybrid physical-chemical vapor deposition. Tunneling from both $\sigma$ and $\pi$ bands of MgB$_2$ to Pb is observed from the current-voltage characteristics (CVCs). The temperature dependence and the magnetic field dependence of the two gaps were obtained by fitting the CVCs in the framework of two band superconductivity. It shows that at zero temperature and zero field, $\Delta_\pi \approx 2.3$ mV and $\Delta_{\sigma} \approx 7.4$ mV. As the applied magnetic field normal to the substrate increases, the contribution from the $\pi$ gap is suppressed much more quickly than the $\sigma$ gap, which is in agreement with lower critical field corresponding to the $\pi$ gap.

$^1$This work is supported by ONR and NSF.

$^{2}$Also with Department of Physics, Beijing University, Beijing, China.

$^3$Also with Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, USA.

8:48AM H8.00003 Mixed State Dissipation in Zero Temperature Limit Enhanced by Two Gap Effect in MgB$_2$ Thin Films. YING JIA, YAN HUANG, HUAN YANG, LEI SHAN, CONG REN, HAI-HU WEN, National Lab for Superconductivity, Institute of Physics, Chinese Academy of Sciences, CHENGGANG ZHUANG, YI CUI, QI LI, XIAOXING XI, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA — Through the measurements of resistive transition, point contact tunneling spectrum and Hall effect on crystalline MgB$_2$ thin films, the dissipation in the mixed state has been exclusively investigated. It is found that the resistive transition broadens monotonously with the magnetic field leading to a non-vanishing mixed state dissipation in zero temperature limit. Hall effect and point contact tunneling measurements indicate that this dissipation is contributed by the vortex motion and associated with the losing of long range phase coherence induced by the proliferation of the quasiparticles from the $\pi$-band. These results suggest the existence of the vortex quantum liquid enhanced by the two gap effect. Some preliminary results on mesoscopic-bridges will also be reported showing the interesting interplay of the two band superconductivity.

9:00AM H8.00004 Observation of the Leggett’s collective mode in MgB$_2$ two-band superconductor$.^4$ G. BLUMBERG, A. MIALITISIN, B. S. DENNIS, Bell Labs, Lucent Technologies, N. D. ZHIGADLO, J. KARPINSKI, ETH, Zurich — We report observation of novel collective mode in the multi-band MgB$_2$ superconductor by resonant electronic Raman spectroscopy. The mode appears below $T_c$, in the $A_{1g}$ scattering channel at 9.2 meV, which is in-between the two gap values, 4.5 meV for the fundamental gap in the $\pi$-band and 13.5 meV for the gap in the $\sigma$-band. We attribute this excitation to collective mode first discussed by Leggett: If a system contains two coupled superfluids a simultaneous cross tunneling of a pair of electrons become possible. The mode is caused by dynamical oscillations of the pairs between the two superfluids leading to small fluctuations of the relative phase of two superconducting condensates. For MgB$_2$ the the oscillations between the condensates involve scattering of a pair of $\sigma$-band electrons with momentum $(k, -k)$ into a pair of $\pi$-band electrons with momentum $(k', -k')$. The symmetry and energy of observed mode is consistent with theoretical predictions.

9:12AM H8.00005 Interplay of ballistic and diffusive superconductivity in the vortex core in the model two-band system MgB$_2$. K. TANAKA, University of Saskatchewan, M. ESCHRIG, Universitaet Karlsruhe, D. F. AGTERBERG, University of Wisconsin - Milwaukee — A revived interest in multi-band superconductivity has emerged due to the unexpected and interesting simultaneous presence of diffusive and ballistic bands in the superconductor MgB$_2$. Motivated by recent experimental data on the vortex state in MgB$_2$ obtained by scanning tunneling spectroscopy, we theoretically study the intriguing effects of superconductivity in a diffusive band (‘$\pi$ band’) induced by superconductivity in a ballistic band (‘$\sigma$ band’). We apply a unique model that has been developed recently$^1$ for describing such a system, based on coupled Eliashberg and Usadel equations. Results are presented for the spatial variation of the order parameter, the current density, and the vortex core spectrum in the two bands. A particularly interesting result emerging from our studies is the possibility of additional bound states near the gap edge in the ‘strong’ $\sigma$ band, which arise from hybridization with the ‘weak’ $\pi$ band. The development of such gap-edge bound states is examined for various sets of physical parameters that are relevant for MgB$_2$. We will also discuss the induced Kramer-Pesch effect in the $\pi$ band and magnetic-field dependence of vortex core size.$^1$ K. Tanaka, D. F. Agterberg, J. Kopu, M. Eschrig, Phys. Rev. B 73, 220501(R) (2006).

9:24AM H8.00006 Breakdown of phase-locked states and limit of the upper critical field controlled by interband scattering in two-gap superconductors. ALEXANDER GUREVICH, National High Magnetic Field Laboratory, Tallahassee, FL 32310, USA — The effect of weak interband scattering on the maximum upper critical field $H_{c2}$, which can be achieved in a two-band superconductor by increasing intraband impurity scattering is considered. Using the two-gap Usadel equations, we show how weak interband scattering provides the crossover from the orbitally limited to the paramagnetically limited $H_{c2}$, both in bulk samples and thin films. The results are applied to describe high $H_{c2}$ values in carbon-doped MgB$_2$ films. It is shown that interband scattering produces mixed gradient terms $\propto Re(\Psi^\dagger \Pi \Psi)$ in the free energy, where $\Pi = \nabla^2 + 2eA/\rho_0$, and $\Psi = \Delta_\sigma \exp(i\theta_\sigma)$ and $\Psi^\dagger = \Delta_\pi \exp(i\theta_\pi)$ are intraband order parameters. The mixed gradient coupling can provide parametric excitation of the plasmon Leggett mode or large-amplitude interband phase textures by ac currents.
9:36AM H8.00007 Effect of oxygen alloying on scattering processes in MgB$_2$, RAGHURAM GANDIKOTA, RAKESH SINGH, YI SHEN, NATHAN NEWMAN, JOHN ROWELL, Arizona State University, ARIZONA STATE UNIVERSITY TEAM — The effect of oxygen alloying on $T_c$, resistivity, $H_{c2}$, and $J_c$ of MBE-grown MgB$_2$ films was studied. Oxygen was introduced either during growth or by ex-situ heating in oxygen atmosphere. While the concentration of oxygen increased from 1 to 9%, $dH_{c2}(0)/dT$ of the films, at $T_c$, increases from 0.67T/K to 1T/K. $J_c$ is greater than 400 kA/cm$^2$ (at 8T, 4.2K) have been observed in these films and increased oxygen alloying changes $J_c$ very little. $H_{c2}^o(0)$ and $H_{c2}^o(0)$ values, obtained in these films with $T_c \sim 31K$, are as high as 43T and 32T respectively. These values are significantly higher than the maximum $H_{c2}^o(0)$ value obtained for ion irradiated films, neutron irradiated MgB$_2$ bulk, and C-allloyed MgB$_2$ bulk. While the $J_c$ values of the oxygen alloyed films are higher than the C-allloyed Penn State films, the $H_{c2}(0)$ values are, however, still significantly smaller than the record values found in the C-allloyed films.

9:48AM H8.00008 MgB$_2$ Tunnel Junctions with Native or Thermal Oxide Barriers, RAGHURAM GANDIKOTA, RAKESH SINGH, YI SHEN, NATHAN NEWMAN, JOHN ROWELL, Arizona State University, ARIZONA STATE UNIVERSITY TEAM — MgB$_2$ tunnel junctions (MgB$_2$/barrier/MgB$_2$) were fabricated using oxides of Mg and stoichiometric MgB$_2$ as the tunnel barrier. The sum of the superconducting gaps ($\Gamma$-gap) observed in conductance-voltage (G-V) measurements was as high as 4.3mV at 4.2 K and a finite value was found for temperatures above 30K. The G-V data exhibit smeared BCS densities of states, indicative of a degraded layer at the electrode/barrier interface. The presence of such an interface might also explain the lack of supercurrents above 20K in junctions exhibiting gap structures above 30K and even in shorted junctions. A subgap current was also observed and was not found to strongly depend on the oxide stoichiometry.

10:00AM H8.00009 Supercconductivity in M$_{n+1}$AX$_n$ compounds, MICHAEL OSOSKY, R. J. SOULEN, JR., S. B. QADRI, Naval Research Laboratory, M. W. BARSOUM, Drexel University, NAVAL RESEARCH LABORATORY COLLABORATION, DREXEL UNIVERSITY COLLABORATION — We present evidence for the presence of bulk superconductivity in several members of the M$_{n+1}$AX$_n$ (M=early transition metal, A=group A element, and X=carbon and/or nitrogen; n=1-3) family of compounds. Samples were synthesized using standard ceramic techniques. We will present resistivity, susceptibility, and specific heat data for these materials. We will also show x-ray diffraction and microscopy data to demonstrate that impurity phases cannot account for the results.

10:12AM H8.00010 Effects of Grain Size and Doping Level on the Critical Current Density of the Ti-sheathed MgB$_2$ Superconducting Wires with SiC Doping, GAN LIANG, HUI FANG, CAD HOYT, Sam Houston State University, Z. P. BUO, Texas A&M University, F. YEN, M. HANNA, A. ALESSANDRINI, K. SALAMA, University of Houston — The effects of the grain size and doping level on the critical current density ($J_c$) of the SiC-doped Ti-sheathed MgB$_2$ superconducting wires were studied. Two groups of samples were prepared: for the first group, the average size of the SiC grains was 20 nm and the doping levels were 5%, 10%, and 15%; for the second group, the doping level of the SiC dopant was 10% and the average sizes of the SiC particles were 20 nm, 43 nm, and 123 nm. All of the samples were sintered at 800°C for 30 minutes. Contrary to the $J_c$ results reported on the SiC-doped Fe-sheathed MgB$_2$ wires by some other groups, we found that the $J_c$ for the SiC-doped Ti-sheathed MgB$_2$ wires decreases with both the increase of SiC concentration and the decay of the grain size. Only for the wires with average grain size of 123 nm, $J_c$ is greater than that of the un-doped MgB$_2$ wires. A simple model is proposed to explain the formation of the impurities in the cores of these doped MgB$_2$ wires. This unusual dependence of $J_c$ on the size and doping-level of the SiC dopant is discussed in association with the magnetization, resistivity, XRD, TEM, and SEM results.

10:24AM H8.00011 Superconducting and Normal State Properties of OsB$_2$, YOGESH SINGH, A. NIAZI, X. ZONG, B.J. SUH, M.W. VANNETTE, R. PROZOROV, D.C. JOHNSTON, Ames Lab. and Phys. and Astron., Iowa State Univ., Ames, IA 50011 — OsB$_2$ is a layered superhard metallic material that was found to superconduct below $T_c = 2.1$ K. We report the first detailed measurements of the static and dynamic magnetic structures $\chi$, electrical resistivity, heat capacity $C_p$, penetration depth, and $^{11}$B NMR on OsB$_2$ to characterize its superconducting and normal state properties. The results confirm that OsB$_2$ is a bulk superconductor below $T_c = 2.1$ K. Its properties can be described by a close to weak-coupling s-wave BCS model with an electron-phonon coupling constant $\lambda = 0.4-0.5$, $\Delta(0)/(k_B T_c) \approx 1.9$, a small Ginzburg-Landau parameter $\kappa$ of order 5 or less, and a small zero-temperature critical field of roughly 300 G. The $^{11}$B NMR measurements in the normal state show a nuclear spin-lattice relaxation time $T_1 = 2.1$ s at room temperature and a Korringa law with $T_1 T = 610$ s K at lower $T$, and a correspondingly small $T$-independent Knight shift. These results indicate a small $s$ character of the conduction electron wave function at the Fermi level. Our results will be compared to corresponding data for MgB$_2$.


1. Supported by NSF Grant DMR-06-03841 and the Alfred P. Sloan Research Foundation.

Tuesday, March 6, 2007 8:00AM - 11:00AM —
Session H9 DMP: Superconductivity: Josephson Junctions, Proximity Effect & Squids I
Colorado Convention Center Korbel 1D

8:00AM H9.00001 Search for second-order Josephson tunneling in Superconductor-Ferromagnet-Superconductor junctions, M.J.A. STOUTIMORE, D.J. VAN HARLINGEN, University of Illinois at Urbana-Champaign, S.M. FROLOV, University of British Columbia, V.V. BOLGINOV, V.A. OBOZNOV, V.V. RAYAZANOVA, Institute of Solid State Physics, Russian Academy of Sciences — We have fabricated Nb-CuNi-Nb SFS (Superconductor-Ferromagnet-Superconductor) superconducting junctions in a geometry that allows us to perform non-uniformity to the junction and the second-order term, proportional to $\sin(2\theta)$, may dominate. The interpretation of past experiments to measure this term have been ambiguous due to concerns that non-uniformity in the ferromagnetic layer could mimic second-order Josephson behavior by producing half-integer Shapiro steps.
8:12AM H9.00002 Superconducting Proximity Effects in Epitaxial Cr/Nb Bi-Layers: A Novel Approach Using a Three-Terminal Device Architecture

This work was supported by NSF.

8:24AM H9.00003 Proximity Effect in Nb/Mg/CoFe Trilayers

8:36AM H9.00004 Proximity effect in superconducting/magnetic nanostructures

8:48AM H9.00005 Effects of magnetic fluctuation on 0-π transition in a superconductor-ferromagnet-superconductor junction

9:00AM H9.00006 Theory of long range superconducting proximity effect in half-metallic ferromagnets: the role of disorder

This work was supported by the DFG via the Center for Functional Nanostructures (M.E.), and by the Alexander von Humboldt Foundation (T.L.), Germany.

9:12AM H9.00007 Electrical Characterization of Superconducting Microbridge Josephson Junctions with Ferromagnetic Strip

9:24AM H9.00008 Long range odd frequency triplet components in F/S/F trilayers

This work was supported by NSF.
behavior of the Josephson barrier will be discussed along with the ramifications for superconductive devices using this technology.

Applications. In the insulating regime that has low Nb concentration, we observe hysteretic junction behavior. Details of the crossover from metallic to insulating achieved. In the metallic barrier regime that has higher Nb content, the uniformity, reproducibility, and tunability have already proven useful for voltage standard applications. In the insulating regime that has low Nb concentration, we observe hysteretic junction behavior. Details of the crossover from metallic to insulating behavior of the Josephson barrier will be discussed along with the ramifications for superconductive devices using this technology.

10:00AM H9.000111 Superconducting Proximity Effect in Thin Semiconducting Films. Michael Vissers, Soren Flexner, Paul Walender, Kevin Underhees, James Eckstein, University of Illinois at Urbana Champaign — The superconducting proximity effect changes both the transport properties of the N-layer as well as the conductance between the N and S layers. We use a novel 3 terminal device structure to probe this which provides two resistance measurements allowing us to measure both the N-layer sheet resistance, Rs, as well as the junction conductance, Gc. When the N-layer is in the metallic regime more than the factor of 2 in Andreev reflection theory predicts, and both Rs as well as Gc exhibit reentrance as a function of temperature. We interpret these changes as the N boundary moving into the semiconductor increasing Gc while simultaneously removing volume in the N-layer that had been used in normal transport. Magnetic fields applied both parallel and perpendicular to the junction cause the maximum conductance to increase while the sheet resistance rises. The magnitude of the necessary field implies a local proximity effect. This work was supported by the DOE BES at the F. Seitz Materials Research Laboratory at the University of Illinois, Urbana.

10:12AM H9.000122 Effect of heavy electron mass m*e on Andreev reflection (AR) in heavy-fermion/superconductor (HF/S) point-contacts. H. Stalzer, W.K. Park, L.H. Greene, Univ. of Illinois at UrbanaChampaign, J.L. Sarrao, J.D. Thompson, Los Alamos Nat. Lab., J. Frederick, P. Canfield, Ames Lab and Iowa State Univ., L.D. Pham, Univ. of California, Davis, Z. Fisk, Univ. of California, Irvine — We investigate the effect of m*e on Andreev reflection in HF/S point-contacts (PC) by measuring the differential electrical conductance at temperatures between 1.5 and 10K. An electrochemically etched Nb tip (Tc = 9.2K) is brought into contact with HF single crystals (CeCoIn5, CeRhIn5, YbAl3) of varying m*e. Our conductance signals show a clear superconducting gap structure expected for PC in the Sharvin regime which can be fitted by the Blonder Tinkham-Klapwijk model. Preliminary results on CeCoIn5 at temperatures above its Tc = 2.3K indicate an enhanced AR signal of similar magnitude as in Au/Nb PC which is in contrast to CeCoIn5/Au PC as reported earlier [1]. We discuss this in the context of a two fluid model which considers heaviness and bandstructure of the HF quasiparticles and which may also explain the asymmetric conductance background observed in many heavy-fermions below a characteristic temperature T*. [1] W. K. Park et al., PRB 72, 052509 (2005). — This work was supported by the Deutsche Forschungsgemeinschaft, and U.S. DoE Award No. DEFGO2-91ER45439 through the FSRMR and the CMM at UIUC and the NSF-DMR-0503360 at UC.

10:24AM H9.000133 Density of States measurements of AlMn alloys with tunable superconducting-gaps. Gálen O’neil, NIST/CU, Dan Schmidt, NIST, Nathan Miller, NIST/CU, Joel Ulloom, NIST, Anthony Williams, Gerald Arnold, Steven Ruggiero, Notre Dame — Superconductors with tunable transition temperatures and energy gaps are useful for a variety of device applications. For instance, transition-edge μ-calorimeter sensors and electron-tunneling μ-refrigerators have been made based on Al with various levels of Mn doping. The transition temperature of AlMn can be continuously tuned from about 1.35 K to below 10 mK by Mn concentrations up to several thousand ppm. Here, we present detailed measurements of the superconducting density of states of AlMn made with both normal metal-insulator-superconductor and superconductor-insulator-superconductor tunnel junctions. For several AlMn approximant compositions, we have measured the hole density of states and the coupling to the Fermi level. In particular, we show that the density of states of AlMn is not gapless as we would expect from magnetic impurities. Rather, present evidence indicates that the density of states is essentially BCS-like with an increased Dynes parameter. The increased Dynes parameter corresponds to a broadened peak at the gap and an increase in subgap states. We discuss the implications of this behavior for tunnel junction devices with AlMn electrodes.

10:36AM H9.000144 Making an Analogy between Forming a Josephson Junction and the Use of Wave Functionals to Form Soliton- Anti Soliton Pairs in Both Biological and Condensed Matter Physics. Andrew Beckwith, APS/ Fermi contractor — Our paper generalizes techniques initially explicitly developed for CDW applications only with respect to what is needed for multi dimensional instantons forming in complex condensed matter and/or bio physics applications. This involves necessary conditions for formation of a soliton- anti soliton pair, assuming a minimum distance between charge centers, and discusses the prior density wave physics example. As the Picek gap term is added to the tilted washboard potential for ensuring the formation of scalar potential fields. We state that the same methodology is needed for higher dimensional condensed matter systems and bio physics, with strict conditions stated as to necessary potential terms needed to form a Josephson junction interpretation as to how to form wave functionals with necessary Gaussian character which can model instanton physics via a process analogous to Piereis gap and Brillouin zone boundary physics.

10:48AM H9.000155 Dynamics of a current-biased Bi2Sr2CaCu2O8+t surface intrinsic Josephson junction. Shaoxiong Li, Wei Qiu, Siyuan Han, Department of Physics and Astronomy, University of Kansas, Y. F. Wei, X. B. Zhu, C. Z. Gu, S. P. Zhao, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, H. B. Wang, National Institute for Materials Science, Tsukuba, Japan — The dynamics of switching from superconducting to voltage state of a current-biased Bi2Sr2CaCu2O8+t surface intrinsic Josephson junction is studied by measuring the temperature-dependent switching current distributions at temperatures ranging from 15 mK to 4.8 K. Crossover from phase diffusion to Kramer switching and thermal activation to quantum tunneling have been observed. Quantitative analysis indicates that the dynamics of a single high Tc Josephson junction can be described very well by theories whose predictions have been confirmed by experiments performed on low Tc Josephson junctions. Our result also indicates that the d-wave order parameter symmetry has no observable effect on the dynamics of Bi2Sr2CaCu2O8+t surface intrinsic Josephson junctions where current is along c-axis of the crystal.

2The work at University of Kansas was supported in part by the NSF Grant No. DMR-0325551 and AFOSR Grant No. F49620-01-1-0439. The work at the Institute of Physics was supported by the NSF of China and the Ministry of Science and Technology of China
8:00AM H10.00001 Ferromagnetism and Glassiness in a Disordered Ising Magnet , C. ANCONA-TORRES, T.F. ROSENSBAUM, University of Chicago, G. AEPPLI, University College London — LiHo$_2$Y$_{1-x}$F$_4$ is a diluted, dipolar-coupled Ising magnet on the boundary between ferromagnet and spin glass. Application of a magnetic field transverse to the Ising axis introduces quantum tunneling modes that speed relaxation and drive an order-disorder transition. We determine the Transverse Field - Temperature phase diagram through measurements of the linear and nonlinear magnetic susceptibility, as well as the spectral response of the system.

8:12AM H10.00002 The Disordered Ising Ferromagnet in Transverse Field , D.M. SILVEITCH, James Franck Institute/University of Chicago, D. BITKO, MPI Research Inc., East Brunswick, NJ, J. BROOKE, Lincoln Laboratory/MIT, G. AEPPLI, University College, London, T.F. ROENSENAU, James Franck Institute/University of Chicago — The phase diagram and critical behavior of the model quantum magnet LiHo$_2$Y$_{1-x}$F$_4$ were studied for $x=0.44, 0.65,$ and $1.0$. Measurements of the phase boundary and critical exponents show mean-field behavior in the classical variable, temperature, but significant deviations from mean-field character emerge in the presence of the quantum variable, transverse magnetic field. Rounding and hysterisis of the magnetic susceptibility in the highly disordered and low temperature limit point to an amplified role for non-equilibrium physics in this regime.

8:24AM H10.00003 Specific Heat of the Dilute Ising Magnet LiHo$_2$Y$_{1-x}$F$_4$ , JEFFREY QUILLIAM, CHAS MUGFORD, LAUREN LETTRESS, JAN KYCIA, University of Waterloo — We will present specific heat results on the dilute dipolar-coupled Ising magnet LiHo$_2$Y$_{1-x}$F$_4$. This material was previously observed to change from a spin glass to an unusual “anti-glass” state at a Ho concentration of $x \approx 0.045$. This state showed dynamics that are very different from those of a spin glass and also exhibited sharp features in its specific heat at around 100 and 300 mK. In contrast, our measurements of the heat capacity do not reproduce these sharp features and instead find broad curves for three concentrations (1.8%, 4.5% and 8.0%). Integrating $C/T$ reveals a residual entropy $S_0$ which is 0 for 8.0% Ho but increases with lower concentration (to 0.31R at 1.8% Ho). This provides some evidence for a change to a different magnetic ground state below 8.0% Ho and is qualitatively consistent with Monte Carlo simulations of AC susceptibility measurements probing the dynamics of this system are currently being performed and results will be presented.

8:36AM H10.00004 Study of magnetism at the atomic level in highly doped LiHo$_2$Y$_{1-x}$F$_4$ , J.A. RODRIGUEZ, A.A. ACZEL, S.R. DUNSIGER, G.J. MACDOUGALL, G.M. LUKE, McMaster University, P.L. RUSSO, TRIUMF, A.T. SAVICI, Brookheaven National Laboratory, Y.J. UMEMU, Columbia University, C.R. WIEBE, Florida State University — LiHo$_2$Y$_{1-x}$F$_4$ is believed to be a physical realization of the ferromagnetic transverse field Ising model. Nevertheless, studies show deviations from the theoretical expectations. One of these differences is the appearance of an anomalous paramagnetic phase after the spin glass state is destroyed by dilution. $\chi_{AC}$ measurements motivated some authors to refer to this phase as an “anti-glass”. Most of the experimental results on the anti-glass phase have been performed at a single Ho concentration ($x = 4.5\%$). In order to better understand the magnetic properties of this system, we performed zero field and longitudinal field $\mu$SR measurements in three highly diluted samples ($x = 0.02, 0.045$ and $0.08$), each of which was expected to lie within the anti-glass phase. Our measurements probe the dynamic behavior of the system in a higher frequency window than the existing $\chi_{AC}$ studies, and have the advantage of being performed with a microscopic probe. We found that there is no qualitative difference on the magnetic behavior upon dilution. In this talk we will discuss the fluctuation of magnetic moments down to base temperature ($\sim 20 mK$) in the presence of a transverse magnetic field. We will also discuss our results on the basis of an independent-ion picture.

8:48AM H10.00005 ABSTRACT HAS BEEN MOVED TO H11.00013 —
9:24AM H10.00008 Magnetic Phase Separation in La$_{1-x}$Sr$_x$CoO$_y$ Single Crystals using $^{139}$La NMR, ROBERT X. SMITH, MICHAEL J.R. HOCH, PHILIP L. KUHNS, WILLIAM G. MOULTON, GREGORY S. BOEBINGER, ARNEIL P. REYES, National Magnet Lab, CHRIS LEIGHTON, Dep. of Chem. Eng. and Mat. Sci., Univ. of Minn, JOHN MITCHELL, Argonne National Lab — Nano-scale phase separation appears to occur in a number of doped transition metal oxides and has been shown to be important in the cobaltites. LSCO is a mixed valence (Co$^{3+}$, Co$^{4+}$) near-cubic perovskite. We report $^{139}$La NMR experiments on nanoscale phase separation in single crystals complementing earlier work on sintered powders$^1$. Concentrations in the range x=0.05 to 0.30, spanning the metal-insulator transition at x=0.18, were used. Spectra for x=0.30 reveal a single peak showing long-range FM order with an internal transferred hyperfine field of 2.5T, at the La site. NMR spectra for samples with x<0.30 show asymmetric peaks that can be well fitted with two Gaussian’s, evidence of FM and spin/cluster-glass magnetic phases. A droplet model has been proposed in the literature, where Co neighbors interact via double exchange in hole-rich regions to form the FM phase. We find magnetic phase separation persists over a narrower x range in the single crystals than in previously studied sintered samples$^1$. 1) M.J.R Hoch et al. PRB 70, 174443 (2004)

9:36AM H10.00009 Spin-glass ordering in the layered III-VI Diluted Magnetic Semiconductor Ga$_{1-x}$Mn$_x$S$^1$. TOM PEKAREK, Univ. of N. Florida, E.M. WATSON, J. GARNER, Univ. of N. FL, P.M. SHAND, I. MIOTKOWSKI, A.K. RAMDAS, Purdue U. — A spin-glass transition has been observed in a class of materials based on a layered III-VI semiconducting host. We have performed dc magnetization and ac susceptibility measurements on the diluted magnetic semiconductor Ga$_{1-x}$Mn$_x$S ($x=0.09$). A scaling analysis of the nonlinear magnetization just above the transition gives $T_c=11.2\pm 0.2$ K, and the critical exponent values gamma = $4.0\pm1.0$ and beta = $0.8\pm0.2$. The non-linear magnetization scaling for Ga$_{1-x}$Mn$_x$S follow the same universal scaling function characterized with the same values of gamma and beta as Zn$_{0.9}$Mn$_{0.1}$Te over many orders of magnitude along each axis. The values for the critical exponents gamma and beta obtained in this work are in excellent agreement with values reported for other spin-glass materials. These results represent convincing evidence that the III-VI diluted magnetic semiconductor Ga$_{1-x}$Mn$_x$S undergoes a true spin-glass transition and is in a subset of the class of insulating spin-glass materials with short-range interactions. The observed spin-glass transition in Ga$_{1-x}$Mn$_x$S is unprecedented in the published literature on III-VI DMS. 1ACs-PRF#40209-5BM, Purdue Univ. Acad. Reinvest. Prog., UNI College of Nat. Sci., NSF DMR-03-05653 & DMR-04-05082.

9:48AM H10.00010 Spin-Glass Like Phase in the Weak-Coupling Limit of the Double-Exchange Model$^1$, RANDY FISHMAN, Oak Ridge National Lab — Recent work has demonstrated that in the weak-coupling or RKKY limit, the double-exchange (or Kondo lattice) model supports a spin-glass like (SGL) phase with short-range but not long-range magnetic order. The magnetic susceptibility and Edwards-Anderson order parameter q of this SGL phase have been evaluated using dynamical mean-field theory (DMFT), which becomes exact in infinite dimensions. We find that q=M(T/T$_{SGL}$)$^2$, where M is the classical Brillouin function and T$_{SGL}$ is the SGL transition temperature. The correlation length of the SGL phase is determined by a correlation parameter Q that simultaneously maximizes T$_{SGL}$ and minimizes the free energy. The magnetic susceptibility has a cusp at T$_{SGL}$ and reaches a nonzero value as the temperature goes to zero. Analytic results for the SGL phase of a model with classical spins but without quenched disorder and geometric frustration should provide new avenues of investigation into SGL behavior.

1Sponsored by Division of Materials Sciences and Engineering, U.S. Department of Energy

10:00AM H10.00011 Chaos in spin glasses, HELMUT G. KATZGRABER, Theoretische Physik, ETH Zurich, FLORENT KRZAKALA, Laboratoire P.C.T., ESPCI Paris — We study the effects of small temperature as well as disorder perturbations on the equilibrium state of three-dimensional Ising spin glasses via an alternate scaling ansatz. By using Monte Carlo simulations, we show that temperature and disorder perturbations yield chaotic changes in the equilibrium state and that temperature chaos is considerably harder to observe than disorder chaos. Results in two space dimensions are also discussed.

10:12AM H10.00012 Spin glass phenomena caused by dipole interactions and the Onsager reaction field , DEREK WALTON, McMaster Un. — The effects of dipole interactions have been the subject of study for decades, however with few exceptions the Onsager reaction field has been neglected. It will be shown that this field leads to waiting time effects and rejuvenation.

10:24AM H10.00013 Universality in spin glasses: A Monte Carlo study, HELMUT G. KATZGRABER, MATHIAS KOERNER, Theoretische Physik, ETH Zurich, A. PETER YOUNG, Physics Department, University of California Santa Cruz — We study universality in three-dimensional Ising spin glasses by large-scale Monte Carlo simulations of the Edwards-Anderson Ising spin glass for several choices of bond distributions, with particular emphasis on Gaussian and bimodal interactions. A finite-size scaling analysis suggests that three-dimensional Ising spin glasses obey universality. Results in two space dimensions are briefly discussed.

Tuesday, March 6, 2007 8:00AM - 11:00AM — Session H11 DMP: Focus Session: Multiferroic Heterostructures Colorado Convention Center Korbel 1F

8:00AM H11.00001 Multiferroic BiFeO$_3$/BiCrO$_3$ superlattices, MARK HUIJBEN, COLLEEN KANTNER, QIAN ZHAN, JOSEPH ORENSTEIN, RAMAMOORTHY RAMESH, Physics Department, University of California, Berkeley — There is currently an increasing interest into multiferroic materials. Although a large number of potential applications can be envisaged, there are currently no known single-phase materials that show large, robust magnetization and polarization at room temperature. Theoretical calculations of artificially constructed (111) layered double perovskite Bi$_2$FeCrO$_6$ predict them to be ferrimagnetic (with a magnetic moment of 2 µB per formula unit) and ferroelectric (with a polarization of ~80 µC/cm$^2$). A high degree of control over the layer composition is required to accomplish this. In this work we fabricated such epitaxial BiFeO$_3$/BiCrO$_3$ superlattices by laser-MBE during which the growth was controlled on the atomic scale by reflection high energy electron diffraction. We will report results of structural, chemical, electrical and magnetic measurements of such superlattices.
8:12AM H11.00002 Electric Field Controlled Magnetism in BiFeO₃/Ferromagnet Films

M. BARRY, K. LEE, Y.H. CHU, P.L. YANG, L.W. MARTIN, C.A. JENKINS, R. RAMESH, UC Berkeley, A. SCHOLL, A. DORAN, ALS/LBNL — BiFeO₃ is the only single phase room temperature multiferroic that is currently known. Not only does it have applications as a lead-free replacement for ferroelectric memory cells and piezoelectric sensors, but its interactions with other materials are now attracting a great deal of attention. Its multiferroic nature has potential in the field of exchange bias, where it could allow electric-field control of the ferromagnetic (FM) magnetization. In order to understand this coupling, an understanding of the magnetization in BiFeO₃ is necessary. X-ray linear and circular dichroism images were obtained using a high spatial resolution photoelectron emission microscope (PEEM), allowing elemental specificity and surface sensitivity. A piezoelectric force microscope (PFM) was used to map the ferroelectric state in micron-sized regions of the films, which were then probed using crystallographic measurements and temperature dependent PEEM measurements. Temperature dependent structural measurements allow decoupling of the two order parameters, ferroelectric and magnetic, contributing to the photoemission signal. Careful analysis of linear and circular dichroism images allows determination of magnetic directions in BiFeO₃ and FM layers.

8:24AM H11.00003 Ferroelectricity in (BaTiO₃)ₙ/(SrTiO₃)ₘ Superlattices Containing as Few as one BaTiO₃ Layer (n=1)

DARRELL SCHLÖM, Penn State University — The question of how thin a ferroelectric can be and still be ferroelectric has been the source of an intensive research effort over the past decade. Several studies, both theoretical and experimental, have concluded that with appropriate boundary conditions ferroelectricity can exist in superlattices containing BaTiO₃ or PbTiO₃ layers as thin as one unit cell. In this talk I will show the results of experiment and theory for BaTiO₃/SrTiO₃ superlattices grown by reactive molecular-beam epitaxy (MBE) on three different substrates: TiO₂-terminated (001) SrTiO₃, (110) DyScO₃, and (110) GdScO₃. With the aid of reflection high-energy electron diffraction (RHEED), precise single-monolayer doses of BaO, SrO, and TiO₂ were deposited sequentially to create commensurate BaTiO₃/SrTiO₃ superlattices with a variety of periodicities. The superlattices consist of n unit-cell-thick slab of BaTiO₃ followed by an m unit-cell-thick slab of SrTiO₃, which are designated [(BaTiO₃)ₙ/(SrTiO₃)ₘ]q, where q is the number of times the bilayer is repeated. X-ray diffraction (XRD) measurements exhibit clear superlattice peaks and the narrowest rocking curves ever reported for oxide superlattices. High-resolution transmission electron microscopy reveals nearly atomically abrupt interfaces. UV Raman results show that the BaTiO₃ in these [(BaTiO₃)ₙ/(SrTiO₃)ₘ]q superlattices is tetragonal and the SrTiO₃ is polar due to strain. Temperature-dependent UV Raman and XRD reveal the paraelectric-to-ferroelectric phase transition temperature (Tc). Our results demonstrate that [(BaTiO₃)ₙ/(SrTiO₃)ₘ]q superlattices containing as few as one strained BaTiO₃ layer (n=1) are ferroelectric and (2) the sensitivity of Tc to the boundary conditions. Comparisons to ab initio and phase-field modeling of the properties of these [(BaTiO₃)ₙ/(SrTiO₃)ₘ]q ferroelectric superlattices will be made and the importance of strain demonstrated. In addition to probing finite size effects and the importance of mechanical boundary conditions, these heterostructures may be relevant for novel phonon devices, including mirrors, filters, and cavities for coherent phonon generation and control. * D.A. Tenne, A. Bruchhausen, N.D. Lanzillotti-Kimura, A. Fainstein, R.S. Katiyar, A. Cantarero, A. Soukiasian, V. Vaiyathan, J.H. Haeni, W. Tian, D.G. Schlom, K.J. Choi, D.M. Kim, C.B. Eom, H.P. Sun, X.Q. Pan, Y.L. Li, Q. Chen, Q.X. Jia, S.M. Nakhmanson, K.M. Rabe, and X.X. Xi, “Probing Nanoscale Ferroelectricity by Ultraviolet Raman Spectroscopy,” Science 313 (2006) 1614-1616.

1The financial support of the Office of Naval Research (ONR) by grants N00014-03-1-0721 and N00014-04-1-0426 monitored by Dr. Colin Wood is gratefully acknowledged.

9:00AM H11.00004 Magnetoelectric Phase Control in Epitaxial Oxides from First Principles

CRAIG FENNIE, Argonne National Lab, KARIN RABE, Rutgers, The State University of New Jersey — We propose a design strategy — based on the coupling of spins, optical phonons, and strain — for systems in which magnetic (electric) phase control can be achieved by an applied electric (magnetic) field. Using first-principles density-functional theory calculations, we present a realization of this strategy for the magnetic perovskite EuTiO₃.

9:12AM H11.00005 Interfacial multiferroism and giant magnetoelectricity in nano-capacitors

JAMES RONDONELLI, MASSIMILIANO STENGEL, NICOLA SPALDIN, Materials Department, University of California, Santa Barbara — We present results of density functional calculations of the dielectric and magnetic responses of SrRuO₃/SrTiO₃/SrRuO₃ oxide heterostructures. Our calculations indicate the spatial coexistence of magnetic and polar behavior at the metal-insulator interface, suggesting a route to a new type of interfacial multiferroic. We also find a giant magnetoelectric response, and comment on the control of this magnetoelectric effect as a means to realizing new devices and sensors. Such devices should be feasible as the ability to fabricate and functionalize new complex materials continues to grow. By controlling the interacting charge, spin and lattice degrees of freedom at interfaces, it is then possible to tune the interactions between layers to create new electric or magnetic phases that are accessible with applied fields.

9:24AM H11.00006 Non-Linear Optical probing of MultiFerroicity and Phase Transitions in BiFeO₃ Thin Films

AMIT KUMAR, Dept. of Materials Science and Engg., Pennsylvania State University, UA, LANE MARTIN, R. RAMESH, Dept. of Materials Science and Engg, University of California, Berkeley, Berkeley, CA, VENKATRAMAN GOPALAN, Dept. of Materials Science and Engg., Pennsylvania State University, UA, PA — Bismuth Iron Oxide BiFeO₃ is being studied extensively by researchers to utilize its multiferroic properties for designing multi-state memory devices. In this work, we present the first results of the non linear optical probing of this material to study the simultaneous ferroelectric and antiferromagnetic ordering below the Neel’s temperature. Optical second harmonic generation (SHG) has been employed to determine crystal and magnetic symmetries of thin BiFeO₃ films grown in different orientations at temperatures ranging from room temperatures to above the Neel’s Temperature. We show that SHG can separate the antiferromagnetic and ferroelectric order parameters cleanly and probe each of these phenomena. The coupling between the ferroelectric and antiferromagnetic ordering under electric and magnetic fields will be presented.

9:36AM H11.00007 Optical spectroscopic study on new magnetoelectric hexagonal REMnO₃ (RE=Gd, Tb, Dy, and Ho) thin films

WOO SEOK CHOI, SUNG SEOK A. SEO, JUNG HYUK LEE, DAESU LEE, TAE WON NOH, ReCOPE & FPDR, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, YUNSANG LEE, Department of Physics, Soongsil University, Seoul 156-743, Korea — Recently, magnetoelectric effects in various oxides have been attracting lots of attentions and are being extensively investigated due to their intriguing couplings between the magnetic and electric order parameters. Here we report optical spectroscopic investigations on new hexagonal REMnO₃ (RE = Gd, Tb, Dy, and Ho) thin films, which are fabricated by epi-stabilization technique [1]. From the in-plane optical conductivity spectra of the hexagonal REMnO₃, we observe a dramatic increase of the optical transition related to Mn 3d a₁g energy level, as the ionic radius of the R ion increases. The optical transition at 1.64 eV for DyMnO₃ shifts to 1.67 and 1.81 for TbMnO₃ and GdMnO₃ respectively. For natural hexagonal REMnO₃ (RE = Y, Er, Lu, and Sc) with smaller ionic sizes, the same optical transitions occur at ~1.6 eV. The large peak shift in new hexagonal REMnO₃ is understood by local flattening of Mn-O bipyrarmid, which will enhance the crystal field energy of a₁g, as the RE ionic size increases.

9:48AM H11.00008 Electronic reconstruction at SrMnO$_3$-LaMnO$_3$ superlattice interfaces . SERB SANDIC, PETER ABBAMONTE, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, IL 61801, USA, ANAND BHATTACHARYA, Argonne National Laboratory, IL 60439, USA, XIAOFANG ZHAI, JAMES ECKSTEIN, FS MRL, UIUC, IL 61801, USA, ANDRIVO RUSYDI, University of Hamburg, D-20355, Germany — Progress in molecular beam epitaxy made possible the growth of manganese oxide superlattices with the dopant ions arranged in separate regular layers. Little is known about how this "structured" doping is reflected into the MnO$_2$ planes; for instance what is the plane effective hole concentration. We studied superlattices made of SrMnO$_3$ and LaMnO$_3$ layers with a doping of x=0.33 using resonant x-ray scattering. For scattering momenta at which the non-resonant contribution is suppressed by symmetry, i. e. L=3 in units of the superlattice period, resonant soft x-ray scattering probes the distribution of doped holes, and, in particular, the nature of the interface between the doped and undoped layers. Our measurements at the O K edge show a temperature-dependent hole distribution. This electronic reconstruction which occurs with cooling below T$_c$=220 K is related to the transition of the superlattice to a ferromagnetic state. Resonant scattering spectra at the Mn L edges from spin and orbital distributions have complex shapes providing additional insights into these new materials.

10:00AM H11.00009 Transport and magnetic properties of digital superlattices of (LaMnO$_3$)$_n$/SrMnO$_3$, . A. BHATTACHARYA, Materials Science Division (MSD), Argonne National Laboratory (Argonne), J. KAVICH, Department of Physics (Physics), University of Chicago (UIUC) and Advanced Photon Source (APS), Argonne, S.G.E. TE VELTHUIS, MSD, Argonne, A. BHATTACHARYA, Materials Science Division (MSD), Argonne National Laboratory (Argonne), J. N. ECKSTEIN, Physics, UIUC — Superlattices of (LaMnO$_3$)$_n$/SrMnO$_3$, $n=1$-$5$, were synthesized using O$_x$-assisted MBE. Both constituents are antiferromagnetic-insulators at low temperatures. The overall stoichiometry is the same as for La$_2$Sr$_{1/3}$MnO$_3$ random alloys, but the $A$-site disorder is eliminated. For $n=1$, 2 a metallic ferromagnetic state is obtained at low T. For $n=1$, all measured properties are nearly identical to those of the random alloy. The emergence of a metallic state is interpreted in terms of a Mott transition driven by the proximity between LaMnO$_3$ and SrMnO$_3$ layers with a doping of x=0.33 using resonant x-ray scattering.

10:12AM H11.00010 Interface Magnetization in Digitally Layered (LaMnO$_3$)$_{2n}$/SrMnO$_3$ Superlattices . J.J. KAVICH, KEVIN SMITH, GUNTER LUEPKE, College of William and Mary — The artificial perovskite superlattices composed of LaMnO$_3$ (LMO) and SrMnO$_3$ (SMO) have been investigated to elucidate the interface ferromagnetic order created by adjoining the antiferromagnetic Mott insulators. Optically-induced coherent spin precessions are studied by time-resolved magneto-optical Kerr effect in a superlattice composed of 4 u. c. unit cells LMO and 2 u. c. SMO for a total of 13 double-layers grown on a single-crystalline (001) substrate of SrTiO$_3$ (STO). We found that the demagnetization field and the anisotropy force are very similar in the LMO/SMO superlattices (H$_d$=0.75 T, H$_a$=0.14 T) and in a La$_{0.7}$Sr$_{0.3}$MnO$_3$ thin film (H$_d$=0.72 T, H$_a$=0.2 T) both grown on STO substrates indicating that the strain and magnetic character are very similar in the two manganite structures. However, the low field precession behavior is distinctly different which shows that pinning by antiferromagnetic spins in the LMO layers and/or surface anisotropy of the superlattice may contribute significantly to the effective field at low applied fields, thus modifying the mode profile and precession frequency. We will discuss this exchange interaction in LMO/SMO superlattices with different periods in zero-field cooling and field cooling.

10:24AM H11.00011 Optically-induced coherent spin precession in manganite superlattices . HAIBIN ZHAO, KEVIN SMITH, GUNTER LUEPKIE, College of William and Mary — The artificial perovskite superlattices composed of LaMnO$_3$ (LMO) and SrMnO$_3$ (SMO) have been investigated to elucidate the interface ferromagnetic order created by adjoining the antiferromagnetic Mott insulators. Optically-induced coherent spin precessions are studied by time-resolved magneto-optical Kerr effect in a superlattice composed of 4 u. c. unit cells LMO and 2 u. c. SMO for a total of 13 double-layers grown on a single-crystalline (001) substrate of SrTiO$_3$ (STO). We found that the demagnetization field and the anisotropy force are very similar in the LMO/SMO superlattices (H$_d$=0.75 T, H$_a$=0.14 T) and in a La$_{0.7}$Sr$_{0.3}$MnO$_3$ thin film (H$_d$=0.72 T, H$_a$=0.2 T) both grown on STO substrates indicating that the strain and magnetic character are very similar in the two manganite structures. However, the low field precession behavior is distinctly different which shows that pinning by antiferromagnetic spins in the LMO layers and/or surface anisotropy of the superlattice may contribute significantly to the effective field at low applied fields, thus modifying the mode profile and precession frequency. We will discuss this exchange interaction in LMO/SMO superlattices with different periods in zero-field cooling and field cooling.

10:36AM H11.00012 Magnetism and electronic structure at the interface of a metal CaRuO$_3$ and Mott insulator CaMnO$_3$ . ALEXANDER BORIS, MPI for Solids, JOHN FREELAND, JERALD KAVICH, ANI, HO NYUNG LEE, ORNL, PETAR YORDANOV, GINIJAT KHALIULLIN, BERNHARD KEIMER, MPI for Solids, JAK CHAKHALIAN, Univ. of Arkansas — Recent advances in fabrication of ultra-thin complex oxide heterostructures have opened new opportunities to investigate possible novel quantum states at the correlated interfaces. Electronic properties of CRO/CMO were investigated by soft x-ray spectroscopies at the L-edges of Mn and Ru. SQUID and optical reflectivity revealed a ferromagnetic-thickness-independent transition at T$_c$≈100K and CRO thickness-dependent negative magnetoresistance. This behavior is marked contrast to the individual layers. At the interface we found a clear sign of net magnetic moment on Mn, which saturates only at magnetic field of 5T. Unlike CMO, similar measurements at the Ru L$_3$-edge showed no detectable magnetism in the field up to 5T. Comparison with Ru references confirmed Ru(IV) oxidation state. These findings are in the sharp contrast with previously suggested models involving Ru(IV-V) valency exchange and thus reveal intricate nature of the interface between a metal and Mott insulator.

10:48AM H11.00013 Probing multiferroicity and spin-spin interactions via angular dependent dielectric measurements on Y-doped HoMnO$_3$ in high magnetic fields . RELJA VASIC, HAIDONG ZHOU, CHRIS WIEBE, JAMES BROOKS, FSU/NHMFL — Dielectric measurements are used to characterize magnetic phase transitions in the doped ferrielectric oxides $Y_x$HoMnO$_3$ (x ∼ 0.4, 0.5, 0.6, 0.7, 0.8, 1.0). The Y Ho$_{1-x}$MnO$_3$ phases exhibit a re-entrant temperature-magnetic field phase transition which involves in-plane Mn spin rotations in the antiferromagnetic state below the Néel temperature are driven by the interaction with the Ho subsystem. We describe this behavior in terms of the interaction of the $Ho$ sublattice spin system with the underlying, robust YMnO$_3$ antiferromagnetic triangular lattice, where the $Ho$-spins interactions are highly sensitive to $Y$ concentration and field direction. The magnetic field anisotropy study is an important step towards understanding of magnetic and electric phase competition in the diluted 4f system by non-magnetic Yttrium($Y$).

---

Tuesday, March 6, 2007 8:00AM - 11:00AM — Session H12 GMAG DMP FIAP: Focus Session: Spin Transport Colorado Convention Center Korbel 3C
8:00AM H12.00001 Dephasing in (Ga,Mn)As Nanowires & Rings1, DIETER WEISS, Experimentelle und Angewandte Physik, University of Regensburg, D-93040 Regensburg, Germany — Quantum correction to the conductivity of ferromagnetic semiconductors are thus far largely unexplored. But to understand quantum mechanical transport the knowledge of basic material properties like phase coherence length and corresponding dephasing mechanism are indispensable ingredients. The lack of observable quantum phenomena prevented experimental access to these quantities so far. Here we report on the observation of universal conductance fluctuations in ferromagnetic (Ga,Mn)As. The analysis of the length and temperature dependence of the fluctuations in one-dimensional wires reveals a 1/T dependence of the dephasing time. The measurement of the Aharonov-Bohm effect in nanowires as well as a weak localization correction to the conductivity, observed in arrays of wires, are in good agreement with the results obtained from the conductance fluctuations.

1Supported by the Deutsche Forschungsgemeinschaft (DFG) via SFB 689 is gratefully acknowledged

8:36AM H12.00002 Low frequency 1/f and random telegraph noise in (Ga,Mn)As1, MENG ZHU, XIA LI, GANG XIANG, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802 — Resistance noise measurements can provide insights into the interplay between charge transport and magnetism in complex physical systems [B. Raquet et al., Phys. Rev. Lett. 84, 4485 (2000)]. We report the temperature- and magnetic field-dependence of the low frequency electrical noise in (Ga,Mn)As epilayers with different Mn concentrations (and different conductivity). Surprisingly, we do not observe any anomalies in the noise spectra across the Curie temperature. However, we find an enhancement in the integrated noise (over the frequency span 125mHz-11Hz) at temperatures below ~ 10 K where the resistivity shows a minimum. For more metallic samples, the normalized power spectrum density is 1/f-like over the entire temperature range studied, while more insulating samples show Lorentzian spectra accompanied by random telegraph noise (RTN) at low temperatures. The magnetic field dependence of the integrated noise shows distinct correlations with magnetization switching, suggesting changes in scattering during domain wall nucleation/propagation. From the magnetic field driven suppression of the RTN, we infer the existence of nanoscale magnetic clusters that fluctuate between two states separated by a field-tunable barrier.

1Supported by NSF and ONR

8:48AM H12.00003 Investigation of Planar Hall Effect in (Ga,Mn)As/GaAs/(Ga,Mn)As Structures, YINGYUAN ZHOU, Z. GE, Y.J. CHO, S. SHEN, X. LIU, J.K. FURDYNA, M. DOBROWOLSKA, Department of Physics, University of Notre Dame, Notre Dame, IN 46556, USA — We present a study of the planar hall effect in the multilayer structures (Ga,Mn)As/GaAs/(Ga,Mn)As. The planar Hall effect (PHE) in a single (Ga,Mn)As layer yields two electric states (high and low), ideal as a basis for device design. The present paper is motivated by the speculation that a coupled (Ga,Mn)As/GaAs/(Ga,Mn)As system provides the possibility of combining PHE with tunneling magnetoresistance, thus leading to complex multiplets of electric states. Our PHE studies were carried out on coupled structures in which the two (Ga,Mn)As layers were made different by either modulation doping or by low temperature annealing. A series of specimens were prepared with different thicknesses of the GaAs spacer (3nm or 6nm). Experimental results show that for samples with 3-nm spacers the magnetic coupling between the two (Ga,Mn)As layers is so strong that their magnetizations reverse together. The PHE then behaves similar to that of a single (Ga,Mn)As layer, except that in the multilayers the PHE voltage switchings are less abrupt. In samples with 6-nm-thick spacer, however, we see the emergence of switchings with multiple values of the PHE voltage. Such multiple electric states can be qualitatively explained by modeling the coupled structures as a network of resistors.

9:00AM H12.00004 Quantum corrections to the longitudinal and anomalous Hall conductivity in (Ga,Mn)As,1, PARTHA MITRA, NITESH KUMAR, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802 — Although the canonical ferromagnetic semiconductor (Ga,Mn)As has now been studied extensively for over a decade, the fundamental understanding of the temperature-dependent conductivity and the origins of the anomalous Hall effect still remain open questions. Here, we report measurements of the longitudinal and transverse conductivity in (Ga,Mn)As samples in the regime of "dirty" diffusive transport. Although we observe a power law temperature dependence of the conductivity, the scaling is inconsistent with standard expectations based upon known quantum corrections to the conductivity. We also examine the scaling of the anomalous Hall conductivity with longitudinal conductivity and compare our observations with theories of the anomalous Hall effect.

1Supported by NSF

9:12AM H12.00005 Magnetotransport and magneto-optical properties of GaMnAs thin films with high Mn concentrations, KENICHI OHNO, Dept. of Electronic Eng., The Univ. of Tokyo, SHINOBU OHYA, Dept. of Electronic Eng., The Univ. of Tokyo; PRESTO JST, MASAKAI TANAKA, Dept. of Electronic Eng., The Univ. of Tokyo; SORST JST — III-V-based ferromagnetic-semiconductor (FMS) GaMnAs is a good model system for future semiconductor-spintronics devices. For practical applications, it is important to increase the Curie temperature (TC) of GaMnAs (the current record is 173 K) to room temperature. The mean field theory predicts that TC of GaMnAs increases in proportion to its Mn concentration x. However, it is difficult to grow GaMnAs with x > 10% because MnAs clusters and Mn interstitial defects are easily formed in such a high x region. Here, we have successfully grown GaMnAs films with x of 12 - 21% by decreasing the growth temperature to 150-200°C and by reducing the film thickness to 10 nm. The magnetic circular dichroism and the anomalous Hall effect measurements indicated that these GaMnAs films have the intrinsic FMS features. A high TC value of 170 K was obtained when x = 12%. This work was partly supported by PRESTO/SORST of JST, Grant-in-aid for Scientific Research, IT Program of RR2002 of MEXT.

9:24AM H12.00006 Electronic transport in diluted magnetic semiconductors: application of the memory function formalism for spin and charge disordered media,1, F.V. KRYCHENKO, C.A. ULLRICH, Department of Physics and Astronomy, University of Missouri - Columbia — To get an expression for electrical conductivity in diluted magnetic semiconductors (DMSs) we employ the memory function formalism and derive a general expression for the current relaxation kernel in spin and charge disordered systems. To illustrate the model we performed simplified calculations of spin and charge scattering rates in the weak-disorder limit for some special cases of interest: (i) In a system with positional correlation of the scattering centers we found a significant enhancement of the charge scattering. The enhancement is sensitive to cluster parameters and may be influenced through post-grow annealing. (ii) In the magnetically ordered system we showed that the suppression of localized spins fluctuations results in the reduction of the spin scattering that substantially contributes to the experimentally observed resistivity drop below TC. (iii) Memory function formalism gives the possibility to include electronic many-body effects in a consistent and systematic manner through time-dependent density functional theory. We use this approach to study the combined effect of disorder and electron-electron interaction on the transport properties of DMSs.

1This work was supported by DOE grant No. DE-FG02-05ER46213.
9:36AM H12.00007 Spin transport through individual single-walled carbon nanotubes SUYONG JUNG, ZHEN YAO, Department of Physics, The University of Texas at Austin, Austin, TX 78712 — We have investigated spin transport through individual single-walled carbon nanotubes contacted with ferromagnetic permalloy electrodes. At low temperatures, hysteretic magnetoresistance (MR) is observed in both the Fabry-Perot interference regime and the Kondo regime. Both the sign and magnitude of the MR oscillate as a function of gate and bias voltages. The behavior in the interference regime can be explained well using non-interacting ballistic model incorporating the effect of spin-dependent interfacial phase shift. In the strongly interacting Kondo regime, however, the behavior of the MR is qualitatively different. We will present possible theoretical models and numerical fittings to elucidate the MR features in our data.

9:48AM H12.00008 Spin transport through Multilayer Graphene1. MASAYA NISHIOKA, ALLEN GOLDMAN, School of Physics and Astronomy, University of Minnesota — We have demonstrated spin valve behavior in structures in which crystals containing multiple graphene layers were positioned between two ferromagnetic contacts. Graphene is a promising candidate for the spacers of spin valves, because of its small spin-orbit interaction and high mobility. We used a 3nm thick crystal which contained several layers of graphene. Cobalt electrodes with a 100nm gap were fabricated on the crystal using electron beam lithography. The device showed ~0.2% magnetoresistance at 10K using an in-plane magnetic field. The effect was found at temperatures as high as 150K. The observed behavior could be explained by the switching of the magnetizations of the Co electrodes, which was inferred from measurements of their anisotropic magnetoresistance.

1Work supported by the National Science Foundation through the University of Minnesota Materials Research Science and Engineering Center under Grant NSF/DMR-0212032.

10:00AM H12.00009 Charge and spin transport in graphene nanostructures, SUNGJAE CHO, YUNG-FU CHEN, MICHAEL S. FUHRER — We have studied spin injection from ferromagnetic (permalloy) electrodes into graphene devices using a non-local four-probe geometry. We observe sign reversal of the non-local resistance upon switching of the magnetization direction of the electrodes, indicating injection and detection of a spin current. We report the temperature and carrier density dependence of the spin valve signal. We observe an unusual reversal of the sign of the spin valve signal at some carrier densities. We have also examined the magnetotransport in the low field and quantum Hall regimes in devices with mobilities differing by an order of magnitude. The results will be discussed in terms of the physics of conduction at the Dirac point. Support provided by the Office of Naval Research and the UMD-MRSEC Shared Equipment Facilities.

10:12AM H12.00010 Magnetoresistance of Gd doped Carbon films, ERIK HELGREN, UC Berkeley, LJ ZENG, UCSD, C. RONNING, U. Gottingen, H. ZUTZ, J. AGER, LBNL, F. HELLMAN, UC Berkeley — The rare earth dopant Gd was introduced into amorphous carbon (a-C) by two quite different techniques; mass selected ion beam deposition (MSIBD) of tetrahedral amorphous carbon (ta-C) followed by Gd implantation and magnetron co-sputtering of Gd and C targets. Raman, RBS and TEM characterization indicate the films are metastable. Films prepared by sputtering (a-Gd, C1−x) with x=4.2-15.6 at.%) have a spin-glass freezing with a temperature which scales with Gd concentration. Films prepared by MSIBD followed by ion implantation (taC:Gd, x=4, 7, 13 at.%) show no freezing and a paramagnetic Curie-Weiss law down to 1.9K. Transport measurements show typical doped amorphous semiconductor behavior with very large negative magnetoresistance (MR). The MR of the two types of films are similar, which indicates a universal magnetic moment-carrier interaction in these Gd doped amorphous semiconductor systems. A comparison of these films’ MR with other Gd doped semiconductors such as a-Gd:Si and a-Gd:Ge will be discussed. The MR properties of this type of thin film material indicate the importance of the local materials structure and the consequence of the electron screening effects.

10:24AM H12.00011 Anti-Weak Localization Measurements in the Ballistic Regime, DILHANI JAYATHILAKA, ARUNA PEDIGAMA, SHEENA MURPHY, MADHAVIE EDIRISOOYI, NITI GOEL, TETSUYA MISHIMA, MICHAEL SANTOS, KIERAN MULLEN, University of Oklahoma, C-SPIN COLLABORATION — Anti-weak localization dominates at low fields in systems in which spin-orbit coupling is strong. The experimental results are well described by theory in low mobility systems in which the magnetic length (λB) is greater than the mean free path; however high mobility systems with strong spin-orbit interactions, such the InSb based two dimensional systems (2DESs) examined here, are not in this diffusive regime. A recent theoretical development [2] addresses both the diffusive and ballistic regimes taking into account both the backscattered and non-backscattered contributions to the conductivity. We will discuss the agreement of the new theory to measurements of InSb 2DES prepared with both strong Dresselhaus and Rashba effects. [1] S.V. Iordanskii, Yu. B. Lyanda-Geller, and G.E. Pikus, JETP Lett. 60, 206 (1994). [2] L.E. Golub, Phys. Rev. B 71, 235310 (2005).

10:36AM H12.00012 Electrical measurement of pure spin currents in a two dimensional electron gas, ANANTH VENKATESAN, SERGEY FROLOV, JOSHUA FOLK, University of British Columbia, Canada, WERNER WEGSCHIEIDER, Universität Regensburg, Germany — We present an electrical measurement of pure spin currents in a AlgAs/GaAs two dimensional electron gas. Spin polarized electrons are injected into the centre of a 90μm long channel through a quantum point contact (QPC) in a large in-plane magnetic field. The charge current flows to one end of the channel. A pure spin current flows to the opposite end, driven by a chemical potential difference between the two spin populations. This difference is recorded using spin polarized QPCs along the channel in regions free of charge current.

10:48AM H12.00013 77Se NMR investigation of the paramagnetic metal phase of λ-(BETS)2FeCl4, GUOQING WU, W.G. CLARK, S.E. BROWN, UCLA Physics and Astronomy, J.S. BROOKS, NHMFL Tallahassee, A. KOBAYASHI, Res Ctr. Spectrochem., Univ. of Tokyo, Japan, H. KOBAYASHI, Inst. Mol. Science, Okazaki, Japan — We report 77Se NMR measurements of the spectrum and the spin-lattice relaxation rate (1/T1) in a 7 μg single crystal of λ-(BETS)2FeCl4 over the temperature (T) range 2.5-10 K in an applied field of 10.9 T parallel to the α-axis (paramagnetic metal phase). A behavior close to 1/T1 = constant is observed. It indicates that for these conditions, 1/T1 is dominated by the hyperfine interaction between the 77Se spins and the conduction electrons, in contrast to 1/T1 for the protons, which is driven by the magnetic fluctuations of the Fe3+ spins [W.G. Clark et al., Appl. Mag. Res. 27, 279 (2004)]. From these proton measurements, we estimate that the contribution of the Fe3+ fluctuations to 1/T1 of 77Se is negligible. Work at UCLA was supported by NSF Grants DMR-0334869 (WGC) and DMR-0520552 (SEB).

Tuesday, March 6, 2007 8:00AM - 10:48AM — Session H13 DMP GMAG: Focus Session: NaCoO2 and AxNiO2 — Colorado Convention Center Korbel 4C
8:00AM H13.00001 Novel sodium ordering on a NaxCoO2 surface. WOEI WU PAI, Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan, S.S. HUANG, Department of Physics, National Normal Taiwan University, Taipei, Taiwan, C.H. LIN, Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan, H. S. HSUE, National Synchrotron Radiation Center, Hsin-Chu, Taiwan, F.C. CHO, Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan — The conducting layered sodium cobaltate, NaxCoO2, has generated great research interests recently. This material exhibits surprising properties as the Na concentration x is varied. Despite intense studies, Na ordering and its subtle interplay with charge ordering in the CoO2 layer remains unclear. Here we report the first direct observation of Na ordering on a NaxCoO2 surface (x=0.84) with scanning tunneling microscopy. Three distinct Na phases, all of hexagonal symmetry, were identified. These new findings did not fit any theoretical prediction at present. Plausible structure models were proposed. In additional, an one-dimensional stripe modulation on the surface was discovered, which was found to be a bulk phenomenon as well. Our results should prompt more detailed theoretical investigations into the mechanism of Na ordering.

8:12AM H13.00002 Electronic Structures of Na in Na_xCoO_2. PAOAN LIN, Institute of Physics, Academia Sinica, Taiwan, D. J. HUANG, National Synchrotron Radiation Research Center, HORNG-TAY JENG, Institute of Physics, Academia Sinica, Taiwan, CHEN-SHING HSUE, Department of Physics, National Tsing Hua University, Taiwan — Sodium cobalt oxides (Na_xCoO_2) have attracted renewed because of their exceptionally large thermoelectric power recent discovery of superconductivity in their hydrated counterparts. In order to investigate the dependence on the doping-concentration for the electronic structures, we have carried out a series of LDA+U Ab initio calculation on sod cobalt oxides (Na_xCoO_2) of various dopings. The calcul results were compared with experimental results of polarization-dependent soft x-ray absorption spectroscopy.

8:24AM H13.00003 Pressure effect on magnetic and structural phase transitions in Na_xCoO_2 (x=0.75, 0.80). O.O. KORNETA, S.O. LEONTSEV, Y.V. SUSHKO, University of Kentucky, R. JIN, B.C. SALES, D. MANDRUS, Oak Ridge National Laboratory — The sodium-rich metallic compounds of Na_xCoO_2 family with x ~ 3/4 are known to exhibit an order-disorder structural transition at ~ 340K and a magnetic transition at ~ 22K. We have performed the magnetization and resistivity measurements under hydrostatic pressure to study both phase transitions in compounds with x = 0.75, x = 0.80. The data established positive pressure dependence of both the structural and magnetic transitions. Positive pressure effect on the Neel temperature suggests that superexchange interactions of localized moments may play an important role in magnetic properties of these materials. Such a conjecture is further supported by the observation of the metal-insulator transition (and its pressure evolution) in interplane resistivity of the x = 0.80 compound. 1

1The work at University of Kentucky was supported by NSF grant DMR 05-02706

8:36AM H13.00004 Weak coupling SDW ground state with strong Fermi surface gapping in Na_xCoO_2, x ~ 0.8. M. BRUEHWILER, B. BATLOGG, S.M. KAZAKOV, J. KARPINSKI, Laboratory for Solid State Physics, ETH Zurich, D. SHEPTYAKOV, Paul Scherrer Institute, Villigen, Switzerland — In Na_xCoO_2 the electrons move on a triangular lattice and in the Na-rich composition range (x > 0.75) form a SDW ground state below T_s ~ 22.5 K with a small ordered moment. We have studied this Fermi surface instability with heat capacity, magnetic and transport measurements on a series of samples with various nominal Na content. The SDW phase is characterized by a jump ∆C at T_s and an associated reduction of the electronic density of states. This removal of DOS has been deduced from the high-temperature value of the Sommerfeld γ and the extrapolation from below 1K to T → 0. Interestingly, the ratio ∆C/(ρT_s) ~ 1.5 is close to the BCS weak coupling value. Even more surprising is the observation that up to ~ 80% of the DOS is removed in this Fermi surface instability. In addition to the gapped electronic excitations the specific heat is measured above γ ~ T ≈ (x ≥ 0.75) form a SDW ground state below T_s ~ 22.5 K with a small ordered moment. We have studied this Fermi surface instability with heat capacity, magnetic and transport measurements on a series of samples with various nominal Na content. The SDW phase is characterized by a jump ∆C at T_s and an associated reduction of the electronic density of states. This removal of DOS has been deduced from the high-temperature value of the Sommerfeld γ and the extrapolation from below 1K to T → 0. Interestingly, the ratio ∆C/(ρT_s) ~ 1.5 is close to the BCS weak coupling value. Even more surprising is the observation that up to ~ 80% of the DOS is removed in this Fermi surface instability. In addition to the gapped electronic excitations the specific heat is measured above γ ~ T ≈ (x ≥ 0.75) form a SDW ground state below T_s ~ 22.5 K with a small ordered moment. We have studied this Fermi surface instability with heat capacity, magnetic and transport measurements on a series of samples with various nominal Na content. The SDW phase is characterized by a jump ∆C at T_s and an associated reduction of the electronic density of states. This removal of DOS has been deduced from the high-temperature value of the Sommerfeld γ and the extrapolation from below 1K to T → 0. Interestingly, the ratio ∆C/(ρT_s) ~ 1.5 is close to the BCS weak coupling value. Even more surprising is the observation that up to ~ 80% of the DOS is removed in this Fermi surface instability. In addition to the gapped electronic excitations the specific heat is measured above γ ~ T ≈ (x ≥ 0.75) form a SDW ground state below T_s ~ 22.5 K with a small ordered moment. We have studied this Fermi surface instability with heat capacity, magnetic and transport measurements on a series of samples with various nominal Na content. The SDW phase is characterized by a jump ∆C at T_s and an associated reduction of the electronic density of states. This removal of DOS has been deduced from the high-temperature value of the Sommerfeld γ and the extrapolation from below 1K to T → 0. Interestingly, the ratio ∆C/(ρT_s) ~ 1.5 is close to the BCS weak coupling value. Even more surprising is the observation that up to ~ 80% of the DOS is removed in this Fermi surface instability. In addition to the gapped electronic excitations the specific heat is measured above γ ~ T ≈ (x ≥ 0.75) form a SDW ground state below T_s ~ 22.5 K with a small ordered moment. We have studied this Fermi surface instability with heat capacity, magnetic and transport measurements on a series of samples with various nominal Na content. The SDW phase is characterized by a jump ∆C at T_s and an associated reduction of the electroni...
9:24AM H13.00008 Charge and spin order on the triangular lattice — Na₅CoO₂ at x = 0.5, SEN ZHOU, ZIQIANG WANG, Boston College — The nature of charge and spin order of strongly correlated triangular lattice fermions is investigated in connection to the unconventional insulating state of Na₅CoO₂ at x = 0.5. We study an extended Hubbard (t-U-V) model of the electron doped Co a₁g band using a spatially unrestricted Gutzwiller approximation. We find a new class of charge and spin ordered states at x = 1/3 and x = 0.5 where the system alleviates antiferromagnetic (AF) frustration via charge inhomogeneity. We show that the $\sqrt{3}a \times 2a$ off-plane Na dopant order at x = 0.5 plays an important but subtle role. It induces weak $\sqrt{3}a \times 1a$ charge order in the Co layer without gapping the Fermi surface and allows successive $\sqrt{3}a \times 1a$ AF and $2a \times 2a$ charge/spin ordering transitions at low temperatures. The nesting with the $2a \times 2a$ hexagonal zone boundary gaps out almost the entire Fermi surface at x = 0.5. We study the phase structure and compare to the findings of recent experiments.

9:36AM H13.00009 High Resolution Scanning Tunneling Microscopy of Na₅CoO₂, M.C. BOYER, W.D. WISE, KAMALESH CHATTERJEE, M.A. ZIMMERMANN, E.W. HUDSON, MIT — Since the 2003 discovery of superconductivity in water doped sodium cobaltate (Na₅CoO₂), many experimental techniques have been brought to bear on not only the superconducting parent state (x ~ 0.3) but on other dopings as well. Unfortunately, scanning tunneling microscopy, which has shown so much success in the study of the related cuprates, has not been as successful in the study of Na₅CoO₂. We will present results from topographic and spectroscopic measurements of Na₅CoO₂ made using our variable temperature scanning tunneling microscope, with a focus on changes observed between 130 K and 4 K.

9:48AM H13.00010 Charge and Spin Order in NaₓCoO₂, TING-PONG CHOI, PHILIP PHILLIPS, University of Illinois — Several experimental puzzles surround the insulating state of NaₓCoO₂: 1) antiferromagnetic order is observed but with a reduced moment $\mu_B = 0.25$, 2) the insulating state occurs at a temperature below which Néel order obtains, and 3) static charge ordering is not seen in all NMR experiments. To address these questions, we focus on controlled calculations of the spin-wave spectrum and the magnitude of the local moment proposed for the insulating state: 1) a charge-ordered state with 4-fold symmetry and 2) charge-ordering state with only 2-fold symmetry. We present a detailed iso-spin/spin coupling model which demonstrates how the charge and spin order are coupled. The phase diagram suggests that the ground state of Na₅CoO₂ should be both charge and spin ordered. Several candidates with different ordering are studied under a generalized spin-wave theory. By comparing the Neutron results with the low energy excitation and the calculated structure factor, we conclude that the ground state of Na₅CoO₂ is charge with 4-fold symmetry and long-range spin order. In this state, we find that a spin moment of $\mu_B = 0.25$ is well described by the experimentally relevant parameters for the exchange couplings.

10:00AM H13.00011 Unusual valency and magnetic order in silver nickelates, SERGEY STREITSOV, Institute of Metal Physics, Ekaterinburg, Russia, M.D. JOHANNES, I.I. MAZIN, Naval Research Laboratory, D.I. KHOMSKII, II. Physikalisches Institut, University zu Köln, Köln, Germany — AgNiO₂ forms as a triangular based layered nickelate, with a structure identical to the well-studied alkali nickelates LiNiO₂ or NaNiO₂, but with a double layer of Ag between the oxide planes. The metallic intercalant ions give rise to highly unusual valence state for silver: Ag¹⁺/²⁺. We show that the reason for the underoxidation is that the two silver ions form extremely strong bonding-antibonding bands, pushing the lowest Ag-s derived band beneath the (filled) O p complex. This additionally preserves metallicity down to the lowest measured temperatures and gives rise to complex, competing magnetic interactions. The resulting spin fluctuations may explain the large discrepancy (too large for phonon renormalization) between calculated and measured linear specific heat coefficients. Our calculations do not support a controversial cooperative Jahn-Teller distortion, but a comparison with calculations and experiments for single-layer AgNIO₂ suggests that magnetically driven charge disproportionation may instead explain the observed structural transition.

10:12AM H13.00012 Structural disorder and magnetic properties of NaNi₀.₅Mn₀.₅O₂ and LiNi₀.₅Mn₀.₅O₂, NATASHA CHERNOVA, MIAOMIAO MA, JIE XIAO, M. STANLEY WHITTINGHAM, Institute for Materials Research, SUNY Binghamton, JULIEN BREGER, JORDI CABANA, CLARE GREY, Department of Chemistry, SUNY Stony Brook — Magnetic properties of layered O(3) compounds LiNi₀.₅Mn₀.₅O₂ and NaNi₀.₅Mn₀.₅O₂, and NaNi₀.₅Mn₀.₅O₂ are studied using AC susceptibility and DC magnetization techniques in order to elucidate magnetic interactions within transition metal (TM) layers and between them in compounds with various TM distributions. In ideal layered NaNi₀.₅Mn₀.₅O₂, antiferromagnetic (AF) ordering transition at 60 K and a spin-flop transition at 5 K in the magnetic field of 2.2 T are found. Upon loss of Na, AF ordering changes with ferrimagnetic, which may be caused by Ni²⁺ migration to the Na layer. LiNi₀.₅Mn₀.₅O₂ with flower or zigzag TM order show ferrimagnetic ordering at around 100 K, and significant magnetization hysteresis below this temperature, indicating presence of Ni²⁺ in the Li layer. Magnetic interactions in all compounds are analyzed and models of spin order at low temperatures are proposed.

3This work is financially supported by the US Department of Energy, Office of FreedomCAR and Vehicle Technologies, through the BATTR program at LBNL.

10:24AM H13.00013 Curie-Weiss metallic state in sodium cobaltates, ILYA VEKHTER, Louisiana State University, CHRISTOPHER HOOLEY, University of St Andrews — One of the most intriguing properties of sodium cobaltates, Na₅CoO₂ is the so-called Curie-Weiss metallic phase appearing at relatively high doping, x = 0.7. It exhibits Curie-Weiss magnetic susceptibility in a metal not far from the onset of antiferromagnetic order. Surprisingly for a layered quasi-two-dimensional structure, the neutron scattering experiments in the ordered state yield comparable in-plane and out-of-plane magnetic susceptibilities. In this work, we study the nature of magnetic transitions in NaₓCoO₂ near the verge of transition to a type-A antiferromagnet. We investigate whether in such a system fluctuations of the in-plane magnetization may give the apparent Curie-Weiss behavior in analogy with the spin-fluctuation theory for itinerant ferromagnets. We consider the effect of the crossover from incoherent to coherent interplane transport on the magnetic susceptibility and discuss the effect of sodium doping.

10:36AM H13.00014 Ferromagnetism, paramagnetism and a Curie-Weiss metal in NaxCoO2, JAIME MERINO, Universidad Autónoma de Madrid, BEN POWELL, ROSS MCKENZIE, University of Queensland — Motivated by the unconventional properties and rich phase diagram of Na₅CoO₂ we consider the electronic and magnetic properties of a two-dimensional Hubbard model on an isotropic triangular lattice doped with electrons away from half-filling. Dynamical mean-field theory (DMFT) calculations predict that for negative inter-site hopping amplitudes (t < 0) and an on-site Coulomb repulsion, U, comparable to the bandwidth, the system displays properties typical of a weakly correlated metal. In contrast, for t > 0 a large enhancement of the effective mass, itinerant ferromagnetism and a metallic phase with a Curie-Weiss magnetic susceptibility are found in a broad electron doping range. The transport and magnetic properties measured in Na₅CoO₂ are consistent with DMFT predictions of a metal close to the Mott insulator and we discuss the role of Na doping in driving the system towards the Mott transition. We propose that the Curie-Weiss metal phase observed in Na₅CoO₂ is a consequence of the crossover from “bad metal” with incoherent quasiparticles at temperatures T>T* and Fermi liquid behavior with enhanced parameters below T*, where T* is a low energy coherence scale induced by strong local Coulomb electron correlations. Our analysis shows that the one band Hubbard model on a triangular lattice is not enough to describe the unusual properties of Na₅CoO₂.

Tuesday, March 6, 2007 8:00AM - 11:00AM — Session H14 GMAG DMP: Focus Session: Exchange Bias Colorado Convention Center Korbel 4D
8:00AM H14.00001 Identification and separation of two distinct contributions to the training effect in polycrystalline exchange biased Co/FeMn bilayers, M.K. CHAN, J.S. PARKER, P.A. CROWELL, C. LEIGHTON, University of Minnesota — We show that polycrystalline Co/FeMn bilayers display two distinct forms of training and qualitatively explain their FeMn thickness ($t_{FeMn}$) dependence. The two types of training can be identified and separated via their distinctive field cycle and $t_{FeMn}$ dependences, and the degree of asymmetry between the ascending and descending branches of the hysteresis loops. Samples were prepared via UHV dc magnetron sputter deposition onto Si/SiO$_2$ substrates at room temperature. The Co thickness was 6 nm while $t_{FeMn}$ was varied between 0 and 20 nm. Upon field cooling, hysteresis loops display two distinct forms of training. The first is a single cycle training accompanied by strong reversal asymmetry. The amount of training and degree of asymmetry are correlated and strongly dependent on $t_{FeMn}$. This effect is due to the biaxial anisotropy of the antiferromagnet$^1$. Subsequent loops are symmetric and exhibit multi-loop training that follows a $n^{-1/2}$ dependence, where $n$ is the loop number$^2$. This effect is attributed to thermally activated depinning of weakly coupled uncompensated interfacial antiferromagnet spins. 1. A. Hoffmann, Phys. Rev. Lett. 93 97203, 2004. 2. D. Paccard, C. Schlenker, O. Massenet, R. Montmory, A. Yelon, Phys. Stat. Sol.16, 301, 1966. This work was supported by the NSF MRSEC program and NSF DMR 04-06029.


8:24AM H14.00003 Magnetic configuration in antiferromagnetically coupled [Co/Pd]$_{15}$/TbFeCo with out-of-plane anisotropy, S.M. WATSON, J.A. BORCHERS, NIST, T. HAUET, S. MANGIN, Nancy University, E.E. FULLERTON, Hitachi Global Storage Technologies — We have used Polarized Neutron Reflectometry (PNR) to investigate the magnetic properties of an exchange-coupled bilayer system with out-of-plane magnetization. These systems show potential for increasing storage densities in magnetic recording media. Magnetization measurements suggest the formation of an in-plane domain wall. The magnetic configuration inside such systems results from the competition between the magnetic field, short-range exchange coupling, and long-range dipolar interactions. This study involved [Co(0.5 nm)/Pd(0.5 nm)]$_{15}$/TbFeCo(25 nm) ($X=3.5, 5, 7, 8$ nm) structures. Both the [Co/Pd] and TbFeCo exhibit strong out-of-plane anisotropy and are exchange coupled antiferromagnetically due to the TbFeCo alloy concentration. The magnitude of exchange coupling between the Co layers may be modified by changing the Pd thickness. PNR measurements, which are sensitive to the in-plane component of the magnetization only, confirm the formation of an in-plane domain wall that varies with the exchange stiffness inside the Co/Pd and with the field. The extent of the in-plane domain wall decreases with increasing applied field for the films with Pd thicknesses of 7 and 5 nm whereas the behaviour of the thinnest film (Pd = 3.5 nm) suggests the Co/Pd bilayers show no evidence of a domain wall.

8:36AM H14.00004 Positive Exchange Bias in GdFe/NiCoO Thin Films, JUSTIN OLAMIT, KAI LIU, UC Davis — Thin films of GdFe/NiCoO are one of the few systems that exhibit positive exchange bias [1-4]. In this study, we show that the positive bias in Gd$_{2}$Fe$_{1-x}$Ni$_{x}$CoO is sensitive to the GdFe composition and the field cooling sequence. In particular, the hysteresis loops are often bifurcated due to the existence of multiple phases: a low anisotropy phase with a single reversal in small fields and a higher anisotropy phase with a single or double loop, depending on the GdFe stoichiometry. In Fe-rich samples, increasing the cooling field causes the low anisotropy phase to shift from negative to positive bias and the double-loop high anisotropy phase to shift toward negative bias. In Gd-rich samples, the low anisotropy phase is always positively biased and the single-loop high anisotropy phase is always negatively biased for all cooling field strengths. These behaviors are a result of the parallel and antiparallel couplings between different magnetic phases of GdFe with the NiCoO layer. [1] J. Nogues, et al., Phys. Rev. Lett. 76, 4624 (1996). [2] S. Mangin, et al., Phys. Rev. B 68, 140404 (2003). [3] X. Ke, et al., Appl. Phys. Lett. 84, 5458 (2004). [4] D. Z. Yang, et al., Phys. Rev. B 71, 144417 (2005).

1Work supported by ACS-PRF and the Alfred P. Sloan Foundation.

8:48AM H14.00005 Exchange bias training effect in Co/CoO heterostructures with variation of the ferromagnetic film thickness, SRINIVAS POLISETTY, TATHAGATA MUKHERJEE, SARBESWAR SAHOO, CHRISTIAN BINEK, University of Nebraska-Lincoln — The exchange bias (EB) training effect is studied in a Co/CoO heterostructure using low temperature longitudinal Kerr rotation. After field cooling the sample to below the Néel temperature of CoO the EB training effect manifests itself by a decrease of the EB field upon cycling the Co film through consecutive hysteresis loops. We explore the temperature dependence of the training effect and its dependence on the Co-thickness, $t_{Co}$. The latter is studied by locally probing the EB in a wedge Co/CoO system. The gradient of the Co film temperature allows to measure local $t_{Co}$-dependence in a range of $\Delta T_{Co} = 23.6$nm varying over the substrate length of 8.5mm. The Co wedge is prepared by MBE taking advantage of the steep decrease of the Co flux when leaving the center of the Co beam. A wedge angle of $1.6 \times 10^{-4}$ is revealed by local small angle X-ray reflectivity. We compare the measured $t_{Co}$-dependence with our phenomenological theory predicting a $t_{Co}^{-1}$-increase of the leading fitting parameter. This behavior is clearly distinguishable from the $1/t_{Co}$-decrease of the equilibrium EB field.

1Financial support by NSF through Career DMR-0547887 and NRI.
9:00AM 14.00006 Tilted cores of magnetic vortices due to exchange bias.  K. Y. GUSLIENKO, Department of Materials Science and Engineering, Seoul National University, South Korea, A. HOFFMANN, MSD and CNM, Argonne National Laboratory — Recently, the influence of exchange bias on magnetic vortices has been investigated experimentally. By generalizing the rigid vortex model, we develop an analytic model of the magnetization reversal in an exchange-biased ferromagnetic dot. We account explicitly for a non-uniformity of the magnetization reversal mode along the direction perpendicular to the layers. This non-uniformity allows the vortex core position to vary throughout the thickness of the ferromagnetic layer. We show that the geometrical confinement in combination with the interface exchange field leads to new asymmetries of the hysteresis loops. Namely, the critical fields for vortex nucleation and annihilation respond differently to the interfacial exchange bias, resulting in an asymmetry of the irreversible parts of the hysteresis loops in addition to the overall shift due to the exchange bias.

1Supported by DOE under contract No. DE-AC02-06CH11357.


9:12AM 14.00007 Controlling the sign of the exchange bias in Fe,Ni$_x$F$_2$/Co and Fe,Zn$_{1-x}$F$_2$/Co bilayers. MIYEON CHEON, ZHONGYUAN LIU, HONGTAO SHI, DAVID LEDERMAN, Department of Physics, West Virginia University — A correlation between the sign of the exchange bias and the sign of the uncompensated magnetization was observed in the Fe,Ni$_x$F$_2$/Co bilayer system. Due to this correlation and the fact that the uncompensated magnetization was reversed at high fields at low temperatures, the sign of the exchange bias was controlled by correlating the sign of the uncompensated magnetization in this system. The dilute antiferromagnet Fe$_{86}$Zn$_{14}$F$_2$/Co system, which was previously shown to also have a large uncompensated magnetization, also showed the same effect but at slightly higher temperatures. Using a micromagnetic simulation program (OOMMF) and comparing to the experimental data, the micromagnetic constants were obtained.

1This work was supported by the National Science Foundation.

2Presently at State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, China

3Presently at Department of Physics, Sonoma State University, Rohnert Park, CA

9:24AM 14.00008 Dynamic enhancement of the exchange bias training effect. SARBESWAR SAHOO, University of Nebraska-Lincoln, ANDRÉAS BERGER, Hitachi Global Storage Technologies, SRINIVAS POLisetty, CHRISTIAN BINEK, University of Nebraska-Lincoln — Exchange bias in coupled magnetic films and its accompanying training effect are fundamental interface phenomena which impact spintronic applications. Training is referred to as a gradual change of the bias field, which evolves upon cycling the soft layer through consecutive hysteresis loops. We report on its dynamic enhancement in exchange coupled bilayers of soft and hard ferromagnetic materials. Dynamic effects are induced with increasing sweep rate of the applied magnetic field from quasi-static to the fully dynamic range. A dynamically generalized theory based on triggered and partially truncated relaxation is in excellent agreement with the data. Remarkable universality of our theoretical approach is evidenced when applying the approach to the dynamic training effect of a conventional exchange bias system involving an antiferromagnetic pinning layer.

1Thanks to NSF through Career DMR-0547887 and NRI for financial support.

9:36AM 14.00009 Exchange bias inducing temperature. ALEXEY DOBRYNIN, RUSLAN PROZOROV, Ames Laboratory and Department of Physics & Astronomy, Iowa State University, Ames IA 50011 — Characteristic temperatures governing behavior of ferromagnetic-antiferromagnetic (F-AF) heterostructures are discussed. The inducing temperature, $T_{ind}$, at which the easy direction of magnetization is established, is in general case different from the maximum temperature at which exchange bias may exist $T_B$ (blocking temperature) and the Néel temperature of the antiferromagnet $T_N$. The case of $T_{ind} < T_N$ suggests presence of a frustrated interfacial AF spin structure in the system, otherwise $T_{ind} = T_N$. If $T_B < T_{ind} < T_N$, the interfacial F-AF interactions are stronger than that between the interfacial AF spins and the rest of the AF part, assuming rotation of those spins during the magnetization reversal. The exchange bias value in this case is determined by the latter AF exchange coupling. In the case of $T_B < T_{ind} < T_N$, the interfacial AF spins stay stable, and the exchange bias field is determined by the interfacial F-AF coupling.

1Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-ENG-82. This work was supported in part by the Director for Energy Research, Office of Basic Energy Sciences.

9:48AM 14.00010 FORC Study of Magnetization Reversal Asymmetry in Fe/FexFe2 Exchange Biased Thin Films. JUSTIN OLAMIT, KAI LIU, UC Davis, ZHI-PAN LI, Cornell University, IVAN K. SCHULLER, UC San Diego — Asymmetric magnetization in Ni/FexFe2 films is due to local incomplete domain walls in the FM parallel to the interface [1, 2]. We have investigated reversal asymmetry in Fe/epitaxial-FexFe2 using a First Order Reversal Curve (FORC) technique [3]. The major hysteresis loop is asymmetrical. Along the decreasing-field sweep of the hysteresis loop, FORC measurements show that the nucleation of domain structures occurs gradually while the domain annihilations are abrupt. However, along the increasing-field reversal, the domain nucleations are abrupt and the annihilations occur gradually. Rotating the AF easy axis away from the applied field shows that the nucleation and annihilation field distributions also have different angular dependences along the field sweeps. These different distributions lead to the asymmetry seen in the shape of the major loop. [1] Li, et al., PRL 96, 217205 (2006). [2] Morales, et al., APL 89, 072504 (2006). [3] Davies, et al., PRB 70, 224434 (2004); APL 86, 262503 (2005); PRB 72, 134419 (2005).

1Work supported by ACS-PRF, Sloan Foundation, and DOE.

10:00AM 14.00011 Magnetic coupling and training effects in Co/NiO/[Co/Pt] structures with orthogonal easy axes. S. ADENWALLA, A. BARUTH, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln — In an attempt to broaden our understanding of the unexpected oscillatory coupling seen in perpendicularly magnetized [Co/Pt]/NiO/[Co/Pt] samples we have investigated a series of Co/NiO/[Co/Pt] samples in which the magnetization lies in-plane and perpendicular to the plane for the Co and [Co/Pt] layers respectively. Although no preferred coupling is expected, we find a coupling that depends on a variety of parameters including strength of an in-plane magnetic field pulse (the “set field”), the number of cycles (the training effect) and the NiO thickness. The strength of coupling, as measured by a shift in the in-plane hysteresis loop, is directly proportional to the in-plane set field, an effect of the nonzero remanence of the [Co/Pt] layer. On training, the coupling strength drops abruptly by a factor of nearly 3 on the first cycle and drops more slowly thereafter. We attribute this to the presence of domains in the [Co/Pt] layer. [1] A. Baruth et al. Phys. Rev. B 74, 054419 (2006).

1 Funded by NSF grant No. MRSEC DMR-0213808
phonon modes. SF output in the reflected direction was detected. Resonant enhancement of the output when the infrared frequency scanned over phonon modes yielded the such phonons. In the experiment, a tunable infrared (together with dependences on input/output polarization combination and crystal orientation, enabled us to examine more closely the symmetry properties of alpha-quartz. As a second-order nonlinear optical process, SF generation is allowed only with phonon modes that are both infrared and Raman active. This, WEI-TAO LIU, Y. R. SHEN, University of California at Berkeley — Sum-frequency vibrational spectroscopy (SFVS) was used to probe optical phonons of materials in its crystalline and amorphous forms, yet it still presents several obscure aspects in its behavior under heating and densification. First-principles simulations of silica glass and quartz are conducted to explain the experimentally observed rapid increase in optical absorption and consequent defect formation. In particular we compare results obtained using the full dielectric matrix and various model dielectric functions. We analyzed the band structure and the absorption spectrum, with focus on the blue shift with respect to density functional theory results, which has been reported in a recent theoretical study [Garbuio et al., Appl. Phys. Lett. 85, 1571 (2004).] [3] O. Hovorka et. al., Appl. Phys. Lett. 89, 142513 (2006).
9:00AM H20.00006 LDA+U Models of Polarons in LaBr3 and CsI1, JOHN JAFFE, SEBASTIEN KERISIT, KEVIN ROSSO, Pacific Northwest National Lab — We describe calculations of the formation and hopping energies of hole polarons (holes self-consistently localized in lattice distortions) in the wide-bandgap ionic materials LaBr3 and CsI. Both one-center (breathing mode) and two center (anion dimer, also known as Vc center) polarons were treated. The LDA+U method based on the VASP code was employed, since standard DFT methods often fail to represent localized electronic states in solids. We used a 72-atom supercell of the UCl3 structure for LaBr3, and a 54-atom CsCl-structure unit cell for CsI. We attempt to correlate differences in electronic transport between these two compounds with different energy nonproportionality behavior that they exhibit as Ce-activated scintillators.

9:12AM H20.00007 Electrostatic resonances and optical responses of cylindrical clusters1, CHUN WING CHOY, The Chinese University of Hong Kong, J. J. XIAO COLLABORATION, K. W. YU COLLABORATION — We develop a Green function formalism (GFF) for computing the electrostatic resonance in clusters of cylindrical particles. In the GFF, we take advantage of a surface integral equation to avoid matching the complicated boundary conditions on the surfaces of the particles. Numerical solutions of the eigenvalue equation yield a pole spectrum in the spectral representation. The pole spectrum can in turn be used to compute the optical response of these particles. For two cylindrical particles, the results are in excellent agreement with the exact results from the multiple image method and normal mode expansion method. The results of this work can be extended to investigate the enhanced nonlinear optical responses of metal-dielectric composites, as well as optical switching in plasmonic waveguides.

9:24AM H20.00008 Crystal and nonlinear optical properties of triphenylguanidine: theory and experiments1, CLÁUDIA CARDOSO, CFC, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, PEDRO SILVA, CEMDRX, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, FERNANDO NOGUEIRA, CFC, Departamento de Física, Faculdade de Ciências e Tecnologia, UNIVERSIDADE DE COIMBRA — Guanidine compounds have attracted much interest due to the donor and acceptor abilities of the nitrogen and their potential nonlinear optical properties. Octopolar molecules are particularly interesting from the point of view of nonlinear optics. Their null dipole moment does not stand as a drawback for its crystallization and still allows the crystal to present large third order susceptibilities if some symmetry requirements are fulfilled. In the present work we focused on the triphenylguanidine (TPG) octopolar molecule and its crystalline forms. We present computational and experimental results both for the isolated molecule and TPG crystals. The structural properties as well as optical spectra and response properties will be presented from the point of view of the requirements to obtain octopolar molecules-based materials with enhanced nonlinear optical properties.

9:36AM H20.00009 Enhanced Luminescence in the Layered Single Crystal Ce[Ag(CN)2]3, CHRISTINE LAROCHELLE, Franklin & Marshall College — Single crystals of the form Ln[M(CN)2]3 (Ln=trivalent rare earth; M=Ag, Au, or both) have a layered structure consisting of alternating layers of M(CN)2− ions and Ln3+ ions. Recent work on this type of crystal has focused on energy transfer from the metal dicyanide donor to the rare earth acceptors, specifically Tb3+, Eu3+, and Sm3+. Crystals of Ln[Ag(CN)2]3 are particularly interesting because they exhibit site-selective excitation. However, the luminescence intensity in these crystals is vanishingly weak at ambient temperatures. We present preliminary luminescence results from a new sample, Ce[Ag(CN)2]3. This crystal displays strong luminescence at all temperatures between 78 K and 295 K, in contrast with all other rare earth dicyanoargentates we have studied. We present steady-state excitation and emission results along with time-resolved measurements of both the cerium doped crystal and the single crystal La[Ag(CN)2]3 for comparison.

9:48AM H20.00010 Polarizability of Optically Trapped Nanorods1, DOUGLAS BONESSI, KEITH BONIN, Wake Forest University, THAD WALKER, University of Wisconsin Madison — We optically trapped C60 polymer nanorods with diameters of 300-500 nm and lengths of 1-3 microns in water in a single beam trap. While in the trap, the nanorods were optically torqued by rotating the plane of polarization of the trapping light. The polarizability of the rod can be found by measuring the rod rotation rate as a function of the polarization rotation rate, and then finding a theoretical fit to this curve that uses a computation of the applied torque as a function of polarizability. We used a discrete dipole approximation (DDA) routine to calculate torques on these trapped C60 rods.

1This research was supported by a grant from Research Corp.
10:00AM H20.00011 Dynamical structure factor of CaF$_2$: Striking coherent dynamical screening of “atomic” Ca-derived excitations . O.D. RESTREPO, M.C. TROPAREVSKY, A.G. EGUILUZ, U. Tennessee and ORNL, B.C. LARSON, J.Z. TISCHLER, ORNL, P. ZSCHACK, Cornell, Y.Q. CAI, H. ISHII, P. CHOW, NSRRC, Taiwan, E.L. SHIRLEY, NIST, C.C. KAO, BNL — We report ab initio calculations of the dynamical structure factor of CaF$_2$ performed together with time-dependent density functional theory, together with non-resonant inelastic x-ray scattering measurements. The “effective” dielectric function has also been determined. The excitations derived from the “atomic” Ca 3p$\rightarrow$ 3d process display a striking wave vector dependence. Such dipole-allowed excitation would be expected to lie at about 27 eV. However, for small $q$’s the leading Ca 3p$\rightarrow$ 3d feature lies at about 35 eV. We demonstrate that this feature corresponds to a collective mode, whose physics embodies a remarkable manifestation of crystal local-field effects induced by charge localization and their interplay with the dynamical screening at the “natural” 3p$\rightarrow$ 3d energy. For intermediate $q$’s, the 27 eV excitation emerges and coexists with the collective mode —thus highlighting the physics of the “atomic” 3p$\rightarrow$3d excitation in the condensed matter environment, which is controlled by dynamical coherent screening. For large $q$’s the Ca-derived spectrum consists of the “single-particle” Ca 3p$\rightarrow$3d excitation, together with the dipole-forbidden Ca 3s$\rightarrow$3d excitation.

10:12AM H20.00012 Vibrational effects on SrTiO$_3$ by K edge X-ray absorption using first-principle methods . SILVIA TINTE, Ceramics Division, NIST, Gaithersburg, MD 20899-8520, ERIC L. SHIRLEY, Optical Division, NIST, Gaithersburg, MD 20899-8441 — Using the Bethe-Salpeter-equation methodology has recently become possible to calculate core and valence excited electronic states and spectra, which are usually computed in the ground-state atomic positions. However, vibrational effects can shift and broaden the spectrum through coupling atomic displacements to electron states and electronic excitations. In this work, we analyze the phonon effects on the Ti 3d states in cubic SrTiO$_3$ by Ti K edge X-ray absorption fine structure using first-principle methods. LDA total energies and coupled electron-hole Bethe-Salpeter equation calculations are performed for different ionic configurations following relevant normal modes of SrTiO$_3$. As result, we obtain gradients of the excited-state energy and electron-phonon coupling coefficients. Our final goal is to include the Franck-Condon effect on the broadening of the calculated spectra.

Tuesday, March 6, 2007 8:00AM - 10:48AM – Session H24 DMP: Molecular Electronics and Quantum Dots Colorado Convention Center 201

8:00AM H24.00001 BREAK –

8:36AM H24.00002 ABSTRACT WITHDRAWN –

8:48AM H24.00003 Thermopower and Electrical Conductance Measurements of Single Molecule Junctions , PRAMOD SANGI REDDY, SUNG-YEON JANG, RACHEL SEGALMAN, ARUN MAJUMDAR, University of California Berkeley — The thermopower and electrical conductance of metal-molecule-metal junctions is studied by trapping single molecules between two gold electrodes with either a temperature differential (thermopower) or voltage differential (electrical conductance) applied across the electrodes. The voltage differential generated due to a temperature differential across a single molecule of Benzenedithiol, Dibenzenedithiol and Tribenzenedithiol trapped between Au electrodes is measured. The sign of the measured thermopower is used to show unambiguously that electrical conduction in these single molecule junctions is p-type (hole). The electrical current in a metal-molecule-metal junction due to a voltage differential of $\sim$100 mV is measured. The effect of molecular structure on electrical conductance is studied by 1) systematically varying the length of aliphatic molecules and aromatic molecules 2) changing the end groups binding to the electrodes 3) by adding substituents to the molecules. It is seen that the electrical resistance of aliphatic and aromatic molecules increases exponentially with length, while there was little effect of end groups and substituents for the molecules that we studied. Further, aromatic molecules are found to be much less resistive than aliphatic molecules of similar length.

9:00AM H24.00004 Quantum Dots Tailored with Conjugated Polymer , JUN XU, ZHIQUN LIN, Iowa State University — Placing conjugated polymers (CPs) in direct contact with a quantum dot (QD) (i.e., preparing QD-CP nanocomposites) carries advantage over cases where QD aggregation dominates. Such QD-CP nanocomposites possess a well-defined interface that significantly promotes the charge or energy transfer between these two components. However, very few studies have centered on such direct integration and QD-CP nanocomposites confined in nanoscopic geometries have never been explored. Here we demonstrate an approach to graft vinyl functionalized poly(3-hexylthiophene) (P3HT) onto aryl-bromide functionalized CdSe QD surfaces. The photophysical properties of nanocomposites in nanoscopic confined geometries are studied.

9:12AM H24.00005 Plasmonically Enhanced Second-Harmonic Generation from Metallic/Organic Hybrid Self-Assembled Films , KAI CHEN, CEMIL DURAK, RANDY HEFLIN, HANS ROBINSON, Department of Physics, Virginia Tech, Blacksburg, VA, 24061 — We have fabricated a new class of second order nonlinear optical materials by combining ionic self-assembled multilayer (ISAM) films with silver nanoparticle arrays in a non-centrosymmetric geometry. These hybrid films exhibit second-harmonic generation (SHG) efficiencies as much as 1600 times larger than unmodified, conventional ISAM films, which makes a three bilayer hybrid film perform at the same level as a micron thick, 700-1000 bilayer film. This was accomplished by using nanosphere lithography to deposit silver nanoparticles on the ISAM film, tuning the geometry of the particles to make their plasmonic resonances overlap the frequency of optical excitation. Even though the enhancement is already large, we suggest that further refinements of the techniques are expected to lead to additional enhancements of similar or larger magnitude.
9:24AM H24.00006 Reversible Photomechanical Switching of Individual Engineered Molecules at a Surface . MATTHEW COMSTOCK, NIV LEVY, ARMEN KIRAKOSIAN, JONGWEON CHO, FRANK LAUTERWASSER, JESSICA HARVEY, DAVID STRUBBE, JEAN FRECHET, DIRK TRAUNER, STEVEN LOUIE, MICHAEL CROMMIE, University of California at Berkeley — We have spatially resolved reversible light-induced mechanical switching in a single organic molecule bound to a metal surface. Scanning tunneling microscopy (STM) was used to image the features of an individual azobenzene molecule on a gold surface before and after reversibly cycling its mechanical structure between trans and cis states via photo-actuation (i.e., photoisomerization). Azobenzene molecules were engineered to increase their surface photomechanical activity by attaching varying numbers of tert-butyl (TB) ligands (“legs”) to the azobenzene phenyl rings. We find that azobenzene molecules lacking TB legs or having only two legs do not switch on a gold substrate under UV irradiation, while molecules synthesized with four TB legs can be photoswitched on gold. STM images of the functionalized molecules show that increasing the number of TB legs “lifts” the azobenzene molecules from the substrate, thereby increasing their photomechanical activity. The reversibility of the photoactuation, along with comparison of experimental data to ab initio simulation of isomerized azobenzene, confirms the photo-induced trans-cis conversion of single molecules.

9:36AM H24.00007 Magnetic Field Effect on Hybrid Exciton in a Quantum Dot Coated by an Organic Shell . JUSTIN ANGUS, QUE HUONG NGUYEN1, Marshall University — We investigate the effect of magnetic field perturbations on the hybrid exciton in a semiconductor quantum dot coated by an organic material. The spatial confinement effect of electron and holes of the heterostructures have been considered together with the quantum confined Zeeman effect and the magnetic confinement. Upon the application of magnetic field the coupling term between the two kinds of excitons increases. An important result is the possibility of tuning the Wannier-Frenkel exciton resonance by applied magnetic fields.

1The corresponding author

9:48AM H24.00008 Theoretical study of photoisomerization of azobenzene derivatives on Au(111)1 . DAVID A. STRUBBE, MATTHEW J. COMSTOCK, NIV LEVY, ARMEN KIRAKOSIAN, JONGWEON CHO, MICHAEL F. CROMMIE, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — Azobenzene and its various substituted derivatives are organic molecules that can be made to photoisomerize reversibly in solution between the cis and trans isomers. Scanning tunneling microscopy (STM) experiments have recently shown that photoisomerization is also possible in vacuum on a Au(111) surface. We use ab initio pseudopotential density-functional theory to confirm and analyze the experimental results by simulating STM images of the isomers, and we also study how the molecules adsorb on the surface and why some azobenzene derivatives can photoisomerize on the surface while others cannot.

1This work was supported by National Science Foundation Grant No. DMR04-39768, by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and by an NSF Graduate Research Fellowship. Computational resources have been provided by NERSC and NACPI.

10:00AM H24.00009 Reliable and Versatile Molecular Electrodes . PAWAN TYAGI, DONGFENG LI, STEPHEN HOLMES, BRUCE HINDS — Further advancements of molecular electronics will require a reliable and easily scalable electrode fabrication scheme with dimensional control to molecular lengths. We have produced versatile molecular junction (MJ) with high yield (90%) long device life (>1year) using simple photolithography and thin film methods. The critical electrode dimension is readily set to the length of a molecule by the thickness of an insulator film at a pattern edge. A variety of MJs were prepared by attaching paramagnetic molecular clusters to span the exposed edge of metal-insulator-metal tunnel junctions. Magnetic (Co, NiFe and Ni) and nonmagnetic (Cu, Pd, Ta and Au) metal electrodes and Al2O3 insulator were utilized. After molecule attachment ~500% increase in current over bare tunnel junction current was observed. Control experiments including the use of neat solvents, using junction widths longer than molecules, use of insulating molecules, and the reversible binding of molecule to top electrode confirm the successful fabrication of molecular electrodes. MJs were photoactive producing ~60mV photo voltage with white light irradiation. Large magneto-resistance effects were seen with magnetic electrodes.

10:12AM H24.00010 Manipulation of Kondo Effect via Two-Dimensional Molecular Self-Assembly . VIOLETA IANCU, APARNA DESHPANDE, SAW-WAI HLA, Ohio University — We report manipulation of a Kondo resonance originated from the spin-electron interactions between a two dimensional molecular assembly of TBrPPP-Co molecules and a Cu(111) surface at 4.6 K using a low temperature scanning tunneling microscope. By manipulating nearest-neighbor molecules with a scanning tunneling microscope tip we are able to tune the spin-electron coupling of the center molecule inside a small hexagonal molecular assembly in a controlled step-by-step manner. The Kondo temperature increases from 105 to 170 K with a decreasing the number of nearest neighbor molecules from six to zero. This Kondo temperature variation is originated from the scattering of surface electrons by the molecules located at the edges of the molecular layer, which reduces spin-electron coupling strength for the molecules inside the layer. Investigations on different molecular arrangements indicate that the observed Kondo resonance is independent on the molecular lattice. This work is financially supported by US-DOE grant DE-FG02-02ER46012.

10:24AM H24.00011 Spatial correlation of photoisomerization of functionalized azobenzene molecules on a surface . NIV LEVY, MATTHEW J. COMSTOCK, JONGWEON CHO, ARMEN KIRAKOSIAN, LUIS BERNIL-BAUTISTA, Dept. of Physics, UC Berkeley ; Mat. Sci. Div, Lawrence Berkeley Natl. Lab, FRANK LAUTERWASSER, JEAN M. J. FRECHET, Dept. of Chemistry, UC Berkeley ; Mat. Sci. Div, Lawrence Berkeley Natl. Lab, DAVID STRUBBE, STEVEN G. LOUIE, M. F. CROMMIE, Dept. of Physics, UC Berkeley ; Mat. Sci. Div, Lawrence Berkeley Natl. Lab — Photoactive azobenzene molecules have great potential for nanoscale opto-mechanical applications. We report a scanning tunneling microscopy (STM) study of the time-dependence of photo-switching tetra-tert-butyl-azobenzene (TTB-AB) molecules on Au(111). “Switched” molecule concentrations were measured as a function of exposure time to various incident light wavelengths until stationary concentrations were reached. We examined the spatial correlations of the photo-switching rates. Scanning tunneling spectroscopy was used to reveal the possible dependence of switching dynamics on the electronic structure of the islands. Implications for organic photoactive devices will be discussed.

10:36AM H24.00012 Electron transport through the building blocks of proteins1 . DAVID CARDAMONE, GEORGE KIRCZENOW, Department of Physics, Simon Fraser University — We investigate two-terminal charge transport through single oligopeptide molecules, thiol-bonded to gold leads. Applying ab initio and semi-empirical techniques, we calculate equilibrium and non-equilibrium results in the Landauer formalism. The conductance and current thus obtained are consistent with the recent experimental results of X. Y. Xiao, B. Q. Xu, and N. J. Tao (J. Am. Chem. Soc. 126, 5370; Angew. Chem. Int. Ed. 43, 6148). This theory furthermore provides a straightforward explanation of the striking current rectification seen in those experiments.

1This work was supported by NSERC and CIAR.
8:00AM H27.00001 Ionic conductance in nanopores, JOHAN LAGERQVIST, University of California - San Diego, MICHAEL ZWOLAK, California Institute of Technology, MASSIMILIANO DI VENTRA, University of California - San Diego — We study ionic transport through nanopores from the perspective of the microscopic electrostatics. We predict the existence of step-like structures in the ionic conductance as a function of both nanopore diameter and ionic concentration. This is due to the formation and breakup of hydration layers around the ions. In bulk water, there are a few of these layers depending on the pore diameter and the ionic concentration. In this talk, we discuss various properties of the hydration layers and the parameter range necessary to experimentally observe quantized conductance of ions through nanopores. Work supported in part by NSF and NIH.

8:12AM H27.00002 Electrophoretic speed of a polyelectrolyte in a nanopore, SANDIP GHOSAL, Northwestern University — A hydrodynamic model for determining the electrophoretic speed of a polyelectrolyte through a nanopore is presented. It is assumed that the speed is determined by a balance of electrical and viscous forces arising from within the pore in the presence of co and counter ions. Further, classical continuum electrostatics and hydrodynamics as well as the mean field description of Poisson-Boltzmann is assumed to be applicable after accounting for Manning condensation on the polyelectrolyte. An explicit formula for the translocation speed as a function of the pore geometry and other physical parameters is obtained and is shown to be consistent with recent experimental measurements on DNA translocation through nanopores in silicon membranes.

8:24AM H27.00003 ABSTRACT HAS BEEN MOVED TO A41.00013

8:36AM H27.00004 ABSTRACT WITHDRAWN

8:48AM H27.00005 Transcription of ribosomal RNA: the role of antitermination of RNA polymerase, STEFAN KLUMPP, TERRY HWA, Center for Theoretical Biological Physics, UC San Diego — The genes encoding ribosomal RNA are transcribed at high rates of 1-2 transcripts per second. These high transcription rates are crucial to maintain the large concentration of ribosomes necessary in fast growing bacteria. To understand how transcription is regulated under these conditions, we developed a model for the traffic of transcribing RNA polymerases (RNAP). Our simulations show that the transcription rate is limited by the elongation stage of transcription rather than by transcript initiation. The maximal transcription rate is severely impaired by RNAP pausing with pause durations in the second range which is ubiquitous under single-molecule conditions. We propose that ribosomal antitermination reduces pauses and thereby increases the transcription rate. This idea is in quantitative agreement with the observed increase of the elongation rate due to antitermination and predicts a two-fold increase of the transcription rate. Antitermination must be highly efficient, since incomplete antitermination with only a few percent of non-antiterminated, i.e. slow, RNAPs completely abolishes its effect. This result suggests that rho-dependent termination may selectively terminate slow RNAPs.

9:00AM H27.00006 Mechanically induced cis to trans reisomerization of azobenzene, ROBERT TURANSKY, MARTIN KONOPKA, IVAN STICH, Slovak University of Technology, DOMINIK MARX, Ruhr Uni-versitaet Bochum — Using density functional techniques we study me-chanoochemistry of the azobenzene molecule. Azobenzene is an optically switchable molecule. Laser light is normally used to achieve molecular switching between the cis and trans isomers. Through the use of realistic gold electrodes used to exert mechanical energy on the molecule bonded between two gold electrodes in static AFM apparatus. Our model consists of two realistic gold electrodes bridged by dithioazobenzene. We find that pulling the transisomer leads just to formation of gold nanowires and mechanical breakage of the electrodes. However, mechanochemistry with modest applied forces leads to cis → trans reisomerization via rotation mechanism. Contrary, use of simple constraints instead of realistic gold electrodes, leads to cis → trans reisomerization, albeit with significantly larger applied forces and via inversion mechanism. Important experimental and theoretical ramifications of these simulations will be discussed.

9:12AM H27.00007 DNA translocation through protein and synthetic nano pores, ANIKET BHATTACHARYA, University of Central Florida — DNA translocation through narrow protein channels is recognized as an important process in biology. Recently it has attracted lot of attention in the biological community following several experiments on DNA translocation through protein nano-pores, and more recently, through synthetic silicon nano-pores. A fundamental understanding is needed for various biological processes, e.g., entry and exit of a DNA in and out of a cell, efficient separation methods for macromolecules, and, possibly fast DNA sequencing. In this talk I will be presenting results for the DNA translocation using a coarse-grained model for an idealized DNA as well as the pore. I will consider several scenarios for the DNA translocation. First, I will show scaling of translocation time of a homopolymer as it escapes from the trans side to the cis side of an idealized thin membrane. Then I will consider DNA dynamics subject to a driving force inside the pore. Next, I will consider heteropolymer threading through a nano-pore. Specifically we will consider both highly ordered and completely random sequences of the chain and relate specific sequences to the distribution of the translocation time and the residence time inside the pore. These studies also will include effects due to different environment on either side of the pore, specific DNA-pore interactions located at selective sites, etc. I will discuss relevance of these simulation results to recent experiments and theoretical models.

9:30AM H27.00008 DNA translocation through protein and synthetic nano pores, ANIKET BHATTACHARYA, University of Central Florida — DNA translocation through narrow protein channels is recognized as an important process in biology. Recently it has attracted lot of attention in the biological community following several experiments on DNA translocation through protein nano-pores, and more recently, through synthetic silicon nano-pores. A fundamental understanding is needed for various biological processes, e.g., entry and exit of a DNA in and out of a cell, efficient separation methods for macromolecules, and, possibly fast DNA sequencing. In this talk I will be presenting results for the DNA translocation using a coarse-grained model for an idealized DNA as well as the pore. I will consider several scenarios for the DNA translocation. First, I will show scaling of translocation time of a homopolymer as it escapes from the trans side to the cis side of an idealized thin membrane. Then I will consider DNA dynamics subject to a driving force inside the pore. Next, I will consider heteropolymer threading through a nano-pore. Specifically we will consider both highly ordered and completely random sequences of the chain and relate specific sequences to the distribution of the translocation time and the residence time inside the pore. These studies also will include effects due to different environment on either side of the pore, specific DNA-pore interactions located at selective sites, etc. I will discuss relevance of these simulation results to recent experiments and theoretical models.

9:42AM H27.00009 DNA translocation through protein and synthetic nano pores, ANIKET BHATTACHARYA, University of Central Florida — DNA translocation through narrow protein channels is recognized as an important process in biology. Recently it has attracted lot of attention in the biological community following several experiments on DNA translocation through protein nano-pores, and more recently, through synthetic silicon nano-pores. A fundamental understanding is needed for various biological processes, e.g., entry and exit of a DNA in and out of a cell, efficient separation methods for macromolecules, and, possibly fast DNA sequencing. In this talk I will be presenting results for the DNA translocation using a coarse-grained model for an idealized DNA as well as the pore. I will consider several scenarios for the DNA translocation. First, I will show scaling of translocation time of a homopolymer as it escapes from the trans side to the cis side of an idealized thin membrane. Then I will consider DNA dynamics subject to a driving force inside the pore. Next, I will consider heteropolymer threading through a nano-pore. Specifically we will consider both highly ordered and completely random sequences of the chain and relate specific sequences to the distribution of the translocation time and the residence time inside the pore. These studies also will include effects due to different environment on either side of the pore, specific DNA-pore interactions located at selective sites, etc. I will discuss relevance of these simulation results to recent experiments and theoretical models.

9:54AM H27.00010 DNA translocation through protein and synthetic nano pores, ANIKET BHATTACHARYA, University of Central Florida — DNA translocation through narrow protein channels is recognized as an important process in biology. Recently it has attracted lot of attention in the biological community following several experiments on DNA translocation through protein nano-pores, and more recently, through synthetic silicon nano-pores. A fundamental understanding is needed for various biological processes, e.g., entry and exit of a DNA in and out of a cell, efficient separation methods for macromolecules, and, possibly fast DNA sequencing. In this talk I will be presenting results for the DNA translocation using a coarse-grained model for an idealized DNA as well as the pore. I will consider several scenarios for the DNA translocation. First, I will show scaling of translocation time of a homopolymer as it escapes from the trans side to the cis side of an idealized thin membrane. Then I will consider DNA dynamics subject to a driving force inside the pore. Next, I will consider heteropolymer threading through a nano-pore. Specifically we will consider both highly ordered and completely random sequences of the chain and relate specific sequences to the distribution of the translocation time and the residence time inside the pore. These studies also will include effects due to different environment on either side of the pore, specific DNA-pore interactions located at selective sites, etc. I will discuss relevance of these simulation results to recent experiments and theoretical models.
9:48AM H27.00008 DNA nucleoside interaction and identification with carbon nanotubes. SHENG MENG, Physics Department, Harvard University, PAUL MARAGAKIS, Dept. of Chem. and Chem. Biol., Harvard University, COSTAS PAPALOUKAS, Dept. of Bio. Appl. & Tech., Univ. of Ioannina, Greece, EFTTHIMIOS KAXIRAS, Physics and Div. of Eng. and Appl. Sci., Harvard University — DNA and carbon nanotubes (CNTs) are prototypical one-dimensional structures. Segments of single-strand DNA are extremely flexible, strongly hydrophilic biopolymers while CNTs are extremely stiff, strongly hydrophobic nanorods. The interaction between DNA and CNTs is being intensely investigated for possible use in, e.g., DNA transporters or biosensors. Recent success in detecting DNA conformational changes and hybridization by near-infrared fluorescence of CNTs or CNT– field-effect transistors has opened the possibility of DNA sequencing through electronic means. Here we investigate the interaction of individual DNA nucleosides with a CNT in vacuum and in the presence of external gate voltage. We propose a scheme to discriminate between nucleosides on CNTs based on measurement of electronic features through a local probe such as scanning tunneling microscopy. We demonstrate through quantum mechanical calculations that these measurements can achieve 100% efficiency in identifying DNA bases. Our results support the practicality of ultrafast DNA sequencing using electrical measurements.

10:00AM H27.00009 Probing the Structure of DNA-Carbon Nanotube Hybrids with Molecular Dynamics Simulations1. ROBERT R. JOHNSON, ALAN T. JOHNSON, MICHAEL L. KLEIN, University of Pennsylvania — DNA-carbon nanotube hybrids (DNA-NT) consist of a single-walled carbon nanotube (SWNT) wrapped with a self-assembled monolayer of single-stranded DNA (ssDNA). Recent experiments involving DNA-NT have shown that this material holds a wide range of technologically useful properties. However, a detailed understanding of its microscopic structure and interactions is lacking. To assist the interpretation of contemporary experiments, we have performed atomistic molecular dynamics (MD) simulations using empirical force fields. MD reveals the nature of the interactions and structural arrangements involved in DNA-NT. We find that the hybrid material spontaneously self-assembles via the attractive π − π stacking interaction between ssDNA nucleobases and SWNT sidewall. Under ambient conditions, ssDNA adopts various wrapping conformations about SWNT including right- and left-handed helices as well as disordered, kinked structures. These conformations are energetically distinct with the compact right-handed helix the most favorable.

1Research supported by NSF Grant No. DMR05-20020 and by the JSTO DTRA and the Army Research Office Grant No. 911NF-06-1-0462.

10:12AM H27.00010 Finite size effect on hydrogen bond cooperativity in (Ala)n polypeptides: A DFT study using numeric atom-centered orbitals. VOLKER BLUM, Fritz-Haber-Institut, JOEL IRETA, MATTHIAS SCHEFFLER — An accurate representation of the energetic contribution $E_{hb}$ of hydrogen bonds to structure formation is paramount to understand the secondary structure stability of proteins, both qualitatively and quantitatively. However, $E_{hb}$ depends strongly on its environment, and even on the surrounding peptide conformation itself. For instance, a α-helical polypeptide $(\text{Ala})_n$ can not be stabilized by its single hydrogen bond, whereas an infinite α-helical chain $(\text{Ala})_{\infty}$ is clearly energetically stable over a fully extended conformation. We here use all-electron density functional calculations in the PBE generalized gradient approximation by a recently developed, computationally efficient numeric atom-centered orbital based code to investigate this H-bond cooperativity that is intrinsic to Alanine-based polypeptides $(\text{Ala})_n (n\in\{1-20,\infty\})$. We compare finite and infinite prototypical helical conformations (α, π, 3_10) on equal footing, with both neutral and ionic termination for finite $(\text{Ala})_n$ peptides. Moderately sized NAO basis sets allow to capture $E_{hb}$ with meV accuracy, revealing a clear jump in $E_{hb}$ (cooperativity) when two H-bonds first appear in line, followed by slower and more continuous increase of $E_{hb}$ towards $n \to \infty$. V. Blum, R. Gehrke, P. Hauv, V. Hauv, M. Scheffler, The FHI Ab Initio Molecular Simulations (aims) Project, Fritz-Haber-Institut, Berlin (2006).

10:24AM H27.00011 Electronic Structure of DNA: A Maximally-Localized Wannier Function Approach. ARASH MOSTOFI, NICOLA MARZARI, Massachusetts Institute of Technology — We combine large-scale, ab initio electronic structure calculations and the maximally-localized Wannier function approach in order to study the electronic properties of DNA strands. By performing full first-principles calculations on stacked DNA base-pairs, we determine the optimally localized, real-space basis set that is able to describe the infinite one-dimensional system efficiently and accurately. This work opens the way to obtaining a detailed understanding of charge transport and conductance in DNA, bringing closer the prospect of engineering its electronic structure for use in nano-electronic circuits and biotechnology applications.

10:36AM H27.00012 Theoretical study the physical contribution to the signal to noise ratio (SNR) and sensitivity of Extraordinary Magnetoresistance (EMR) quantum well structures1. Y. SHAO, S. A. SOLIN, Washington University in St. Louis, A. GIRGIS, L. R. RAM-MOHAN, Worcester Polytechnic Institute, KEON-HO YOO, Kyung Hee University, Korea — The application of EMR sensor performance requires ultra-thin films with very high mobility $\mu$ and high electron concentration $n$, because the sensitivity of the EMR device is proportional to the $\mu^2$ and the SNR depends on the $n_{2DEG}^{1/2}\mu^{1/2}$ (1/f noise) or $n_{2DEG}^{1/2}\mu^{3/2}$ (thermal noise). We have modeled the electron concentration and mobility in a two dimensional electron gas (2DEG) layer located in a delta-doped InSb/AlInSb heterostructure. The non-parabolic band structure due to the nature of the small energy band gap of InSb is explicitly accounted for. The subband energy levels, electron wave functions and band-edge profiles were obtained using the k $\cdot$ p method. The electron transport properties were calculated by including contributions of scattering from ionized impurities, the background neutral impurities, the deformation potential acoustic phonons, and the polar optical phonons. We have calculated the dependencies of $\mu^2$, $n_{2DEG}^{1/2}\mu^{1/2}$ and $n_{2DEG}^{1/2}\mu^{3/2}$ on temperature, spacer layer thickness, doping density, and the quantum well thickness. This work will impact EMR sensor design.

1Supported by the NSF, the NIH, and the WU CML.

Tuesday, March 6, 2007 8:00AM - 11:00AM –
Session H28 DMP: Focus Session: Graphene I — Colorado Convention Center 302
8:00AM H28.00001 Theory of quantum transport in graphene and nanotubes , TSUNEYA ANDO, Department of Physics, Tokyo Institute of Technology — In graphene, electronic states are described by Weyl’s equation for a massless neutrino [1,2]. The system has a topological singularity at the origin of the wave vector \( \mathbf{k} = 0 \), giving rise to nontrivial Berry’s phase when \( \mathbf{k} \) is rotated around the origin [3]. The singularity causes various zero-mode anomalies such as discrete jumps in the diagonal [4], off-diagonal Hall [5], and dynamical conductivity [6] at the Fermi energy corresponding to \( \mathbf{k} = 0 \). In the presence of a magnetic field, a Landau level with zero energy exists independent of the strength of the field [7], giving rise to a singular diamagnetism of graphene and the large magnetic anisotropy of the carbon nanotube [8] used extensively for the observation of the Aharanov-Bohm effect [9,10]. In the absence of a magnetic field, the system belongs to a symplectic universality class even in the presence of scatterers unless their potential range is smaller than the lattice constant. Being combined with the presence of an odd number of current carrying channels, this leads to the absence of backward scattering [11] and the presence of a perfectly conducting channel [12], making a metallic carbon nanotube a perfect conductor with ideal conductance exhibiting intriguing frequency dependence [13,14]. In the presence of scatterers with range smaller than the lattice constant, the system crossovers from the symplectic to an orthogonal class [15,16], and to a unitary class if higher order \( \mathbf{k} \cdot \mathbf{p} \) terms causing trigonal warping are considered [17] or in magnetic fields [18]. These symmetry crossovers manifest themselves as strong difference in localization effects due to disorder in both graphene [18,19] and a carbon nanotube [20].


8:36AM H28.00002 Charge-Tunable Electron-Phonon Coupling in Single Layer Graphene , JUN YAN, YUANBO ZHANG, PHILIP KIM, ARON PINCZUK, Columbia University — We report the observation of electron-phonon coupling in single layer graphene via gate-modulated Raman spectroscopy. The doubly-degenerate long-wavelength optical phonon of graphene (the G-band) is found to be very sensitive to charging of the single atomic layer by the electric-field-effect. The functional dependences of frequency and line-width on gate voltage are explained in terms of charge-tunable interactions of G-band phonons with particle-hole transitions across a vanishing band gap. The phonon dynamics uncovers, from a unique perspective, the intriguing physics of Dirac fermions residing in this two dimensional hexagonal lattice of carbon atoms. The striking symmetry manifested in the spectra offers an optical venue for the determination of the charge-neutral Dirac-point.

8:48AM H28.00003 Electron-Phonon Interactions in Graphene and Graphene Layers , JIA-AN YAN, W.Y. RUAN, M.Y. CHOU, Georgia Institute of Technology — We have performed first-principles calculations of the phonon linewidth due to the electron-phonon coupling in one and two layers of graphene using the density-functional perturbation theory. For single-layer graphene, we find that the calculated linewidth is dominated by electron interaction with the two highest optical phonon modes near the \( \Gamma \) point and by the highest optical phonon mode near the Brillouin zone boundary corners \( K \) and \( K' \). A value of the mass enhancement parameter, \( \lambda = 0.3 \), is obtained for the one layer when we extrapolate the smearing temperature to zero. As for the case of bilayer graphene, although the phonon dispersion relations are almost identical to those of single layer, significant enhancement of electron interaction with some phonon modes is observed due to interlayer coupling, leading to distinct phonon linewidths.

9:00AM H28.00004 Electron-phonon interaction and valley splittings in graphene , W. Y. RUAN, JIA-AN YAN, LI YANG, M. Y. CHOU, School of Physics, Georgia Institute of Technology — Based upon first-principles calculations, a two-valley effective mass theory has been developed for graphene in a strong magnetic field and the electron-phonon couplings calculated using density-functional perturbation theory. We showed that the electron interaction with phonons about the Brillouin zone corners can lead to valley-splittings which increases linearly with the magnetic field, in agreement with a recent experimental observation.

9:12AM H28.00005 Electron Self-Energy Corrections to Quasiparticle Excitations in Graphene and Large Diameter Single-Walled Carbon Nanotubes , JACK DESLIPPE, DAVID PRENDERGAST, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Recent experimental measurements of the band structure and band velocity at the Dirac point in graphene highlight many novel effects due to the existence of Dirac fermions in this system. The low energy electronic states are measured to have Fermi velocity of approximately \( 1.1 \times 10^6 \text{m/s} \), with energy dispersion obeying the 2D massless Dirac equation. Motivated by this work, we explore in detail the importance of an accurate description of the electron self-energy in determining the quasiparticle band structures of graphene, graphite, and armchair single-walled carbon nanotubes near the Fermi energy, using the GW approximation to the electron self energy. This work was supported by National Science Foundation Grant No. DMR04-39768 and by the US DOE under Contract No. DE-AC02-05CH11231. Computational resources were provided by SDSC and NERSC. Jack Deslippe acknowledges funding from the DOE Computational Science Graduate Fellowship (CSGF).

9:24AM H28.00006 Direct observation of Landau levels of massless and massive Dirac fermions , GUOHONG LI, EVA Y. ANDREI, Dept. of Physics Rutgers University, Piscataway NJ — The low energy quasiparticles in graphene resemble massless relativistic particles (Dirac fermions): they have a linear energy-momentum spectrum and possess internal degrees of freedom arising from the crystal symmetry of the honeycomb lattice, leading to particle anti-particle pairs. When two layers of graphene are coupled together, the quasiparticles acquire a band-structure and are transformed into chiral massive fermions. Both types of quasiparticles develop unusual Landau levels in a magnetic field which profoundly alter the magneto-transport properties. We will report the direct observation of the Landau levels associated with these quasiparticles using a low temperature STM in fields up to 12 Tesla. The experiments reveal two independent sequences of Landau levels that provide evidence for the coexistence of massless and massive Dirac fermions. The energy levels of the former exhibit a square-root dependence on both field and Landau-level index \( n \), while the latter are linear in field with a Landau-level index dependence of \( |n(n+1)|^{1/2} \). Both sequences exhibit a zero energy Landau level which is a unique and direct consequence of the quantum-relativistic nature of these quasiparticles.

1Now supported by DOE DE-FG02-99ER45742 and by NSF-DMR-0456473.

1This work is supported by NSF-DMR.

9:48AM H28.00008 Spin density wave formation in graphene facilitated by the in-plane magnetic field. SEBASTIAN REYES, Stony Brook University and Brookhaven National Laboratory, ALEXEI TSVELIK, Brookhaven National Laboratory — We suggest that by applying a magnetic field lying in the plane of graphene layer one may facilitate an excitonic condensation of electron-hole pairs with opposite spins and chiralties. The provided calculations yield a conservative estimate for the transition temperature $T_c \sim 0.1 B$.

10:00AM H28.00009 Is Graphene a Fermi Liquid?2, WANG-KONG TSE, SANKAR DAS SARMA, EUYHEON HWANG, University of Maryland — In this talk, we answer the question posed in the title above by considering theoretically the electron-electron interaction induced many-body effects in undoped (‘intrinsic’) and doped (‘extrinsic’) 2D graphene layers. We find that (1) intrinsic graphene is a marginal Fermi liquid with the imaginary part of the self-energy, $\Im \Sigma(\omega)$, going as linear in energy $\omega$ for small $\omega$, implying that the quasiparticle spectral weight vanishes at the Dirac point as $|\ln \omega|^{-1}$; and, (2) extrinsic graphene is a well-defined Fermi liquid with $\Im \Sigma(\omega) \sim \omega^2 \ln \omega$ near the Fermi surface similar to 2D carrier systems with parabolic energy dispersion. We provide analytical and numerical results for quasiparticle renormalization in graphene, concluding that all experimental graphene systems are ordinary 2D Fermi liquids since any doping automatically induces generic Fermi liquid behavior.

2This work is supported by US-ONR.

10:12AM H28.00010 Inelastic Coulomb scattering of 2D graphene1, EUYHEON HWANG, B. Y. K HU, SANKAR DASSARMA, University of Maryland at College Park — The inelastic quasiparticle lifetime of 2D graphene is calculated using the full dynamically screened Coulomb interaction. We calculate the imaginary part of the quasiparticle self-energy for doped (or gated) graphene, using the $G_0 W$ and random phases approximations. At low energy regimes, the intraband single particle excitation (SPE) and plasmon contribute to the self energy, but the interband SPE does not contribute to the self energy due to the phase space restrictions. At higher energies ($\omega \gtrsim E_F$) interband SPE contribution increases sharply, overwhelming the intraband SPE and plasmon contribution. The calculated inelastic quasiparticle lifetime is significantly different from semiconductors with parabolic bands because of linear energy dispersion and chiral properties of graphene.

1This work is supported by US-ONR.

10:24AM H28.00011 Evidence for weak antilocalization in epitaxial graphene1, XIAOSONG WU, XUEBIN LI, ZHIMIN SONG, CLAIRE BERGER, WALT A. DE HEER, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 — Transport in ultrathin graphite on silicon carbide is graphene-like and appears to be dominated by the electron-doped epitaxial graphene layer at the interface. Weak antilocalization in 2D samples manifests itself as a broad cusp-like depression in the longitudinal resistance for magnetic fields $10 \text{ mT} < B < 5 \text{ T}$. An extremely sharp weak-localization resistance peak at $B = 0$ is also observed. These features quantitatively agree with recent graphene weak-localization theory. Scattering contributions from charges in the substrate and from trigonal warping due to the graphite layer are tentatively identified. The Shubnikov-de Haas oscillations show an anomalous Berry’s phase. Their small amplitudes may be related to graphene scattering processes.

1Supported by NSF grant 0404084, U.S. Department of Energy grant DE-FG02-02ER45956, a grant from Intel Research Corporation, and a USA-France travel grant from CNRS.

10:36AM H28.00012 Spin-polarized states in zigzag-edge graphene nanostrips1, JOHN W. MINTMIRE, JUNWEN LI, Oklahoma State University, DANIEL GUNLYCKE, CARTER T. WHITE, Naval Research Laboratory — Zigzag-edge graphene nanostrips (GNSs) are known to exhibit localized edge states in the vicinity of the Fermi level. It has previously been reported that these edge states are ferrimagnetic. We present a study based on first-principle DFT and Hubbard model calculations that confirm the ferrimagnetic nature of the edge states. By comparing the results, we have estimated the Hubbard $U$ to be approximately $2.7 \text{ eV}$. Energy dispersions, spin polarizations, and total energies are calculated for various widths of the nanostrips. In both our approaches, we find that the ferrimagnetic states have lower energy than the spin-restricted solution.

1This work was supported by the NRC, ONR, and DoD HPCMO CHSSI program.

10:48AM H28.00013 Study of spin-polarized transport in layers of graphene1, W.-H. WANG, Department of Physics and Astronomy, UC Riverside, K. PI, H. CHOI, P. WEI, J. SHI, R. KAWAKAMI, DEPARTMENT OF PHYSICS AND ASTRONOMY, UC RIVERSIDE COLLABORATION — Electron transport in graphene layers has drawn great attention recently due to the observation of 2D behavior and relativistic dispersion in these systems. Our attention is focused on spin-polarized transport in ferromagnet(FM)/graphene/FM devices in which the FM electrodes act as spin injectors and spin detectors. Specifically, the spin-polarized transport across graphene should be manifested as a dependence of resistance on the relative alignment of the FM electrode magnetizations (i.e. spin valve effect). Few-layer graphene (FLG) are extracted from kish graphite by sonication. FLGs are then dispersed and dried onto SiO2/Si substrate with pre-patterned electrodes. Atomic force microscopy, scanning electron microscopy and optical microscopy are used to characterize topographic properties and surface quality of FLG. FM electrodes are fabricated onto selected FLG using a combination of electron beam lithography and molecular beam epitaxy deposition in ultrahigh vacuum to ensure high quality magnetic materials and interfaces. We have performed initial electrical measurements and results from our studies will be discussed.

1Supported by ONR, NSF, and CNID.

Tuesday, March 6, 2007 8:00AM - 11:00AM –
Session H43 FIAP DMP: Focus Session: Physics of Thermoelectric Materials and Phenomena II
Colorado Convention Center 506
8:00AM H43.00001 Solid State Thermionic Energy Conversion 1. ALI SHAKOURI, University of California Santa Cruz — An overview of the activities at the Thermionic Energy Conversion Center will be given. This is a consortium of twelve research groups that are working to optimize thermoelectric properties of embedded metallic nanoparticles and multilayers. Hot electron filtering using heterostructure barriers is used to break the trade off between high Seebeck coefficient and high electrical conductivity. Embedded ErAs nanoparticles and metal/semiconductor multilayers are used to reduce the lattice thermal conductivity without significant effect on electrical conductivity. The implication of the superlattice transport on the electronic thermal conductivity and Lorenz number will also be discussed. Cross-plane and in-plane thermoelectric properties are characterized in a wide temperature range. The effective ZT of the thin film is measured using the transient Harman technique. Integrated circuit fabrication techniques are used to transfer the n- and p-type thin films on AlN substrates and make power generation modules with hundreds of thin film elements. Potential for energy conversion efficiency exceeding 20% and high power density >1W/cm² will be discussed.

1Work supported by ONR MURI Thermionic Energy Conversion Center

8:36AM H43.00002 High temperature cross-plane Seebeck coefficient measurement of ErAs:InGaAs/InGaAlAs superlattice 1. ZHIXI BIAN, MONA ZEBARJADI, ALI SHAKOURI, University of California, Santa Cruz, GEHONG ZENG, University of California, Santa Barbara, JOHN BOWERS — The 3ω technique is used to measure the Seebeck coefficient across 2 micron superlattices made of 80×((InGaAs)0.9(InAlAs)0.1)-10nm / InGaAs-20 nm films lattice matched to InP substrate. ErAs nanoparticles are randomly distributed within the 20 nm InGaAs layer. We characterized 4 concentrations with different doping concentrations (from 2×10^{18} cm^{-3} to 10^{20}cm^{-3}) in a temperature range of 300K to 600 K. A significant increase in the cross plane Seebeck coefficient compared to the in plane one is observed. Comparison with DC measurement shows that the 3ω method is more accurate especially at high temperatures. Further infrared studies will be carried out to understand the origin of the coupled Schrodinger and Poisson equations, together with modified Boltzmann transport equation is used to explain the experimental results.

8:48AM H43.00003 Electronic Properties of Layered Cobaltates. QING JIE, QIANG LI, Brookhaven National Laboratory — Electronic properties of layered cobaltates are strikingly different from those in conventional metals, that result in water-induced superconductivity and large thermoelectric power factor. Here we report a transport study of thermoelectric power and electrical conductivity as a function of temperature and magnetic field in several cobaltate single crystals and thin films: Ca_{3}Co_{2}O_{5} and highly doped Na_{9}CoO_{2}. There are three temperature regions where the electronic transport properties of these cobaltates exhibit distinctive behaviors. At low temperatures, the transport property is strongly influenced by the magnetism. At the elevated temperatures, it shows the feature of a correlated metal. At high temperatures, it has weak temperature dependence. These results will be compared with the infrared studies.

9:00AM H43.00004 Crystal Structure of Misfit Thermoelectric Compound [Ca_{3}Co_{2}O_{5}]_{0.62}CoO by Electron Diffraction and High Resolution Electron Microscopy. P. OLENYIKOV, V. VOLKOV, Q. JIE, Q. LI, Y. ZHU, Brookhaven National Laboratory, CFN-MSD/BNL TEAM — Layered cobaltates are of great interest from a physics point of view, as shown by their thermoelectric and magnetoresistance properties. In order to understand the origin of physical properties of layered cobaltates and, in particular, of misfit cobalt oxide [Ca_{3}Co_{2}O_{5}]_{0.62}CoO with high thermoelectric power, an accurate determination of the crystal structure is required. Ambiguities of the structure analysis of this compound performed by X-ray methods stimulated us to re-examine its structure by the electron diffraction patterns (DP) and high resolution electron microscopy (HREM) methods. Single crystal [Ca_{3}Co_{2}O_{5}]_{0.62}CoO grown under SrCl2-flux has a misfit lattice structure with rock-salt type [Ca_{3}Co_{2}O_{5}] slabs and interpenetrating CdI2-type [CoO2] layers stacked along c-axis and incommensuration along b-axis. The nearest commensurate structure with ratio of sublattice parameters f1/f2 = 5.8 closely matches the 0.62 composition index. Analysis of HREM images and the presence of lines with diffuse scattering and weak spots on the (h01) DP lead to the tripled a unit cell parameter, which was significantly different from the average structure determined by X-ray and neutrons. Work supported by the U.S. DOE, BES (DE-AC02-98CH10886).

9:12AM H43.00005 Infrared Studies of Charge Dynamics in Ca_{3}Co_{2}O_{5} Thin Films and Single Crystals 1. JIUFENG TU, ZHIJUN XU, The City College of New York, WEIDONG SI, QIANG LI, Brookhaven National Laboratory — In recent years, the 2D-layered cobaltates have emerged as promising p-type thermoelectric materials. These systems show high thermoelectric figure of merit and are ideal candidates as the materials of choice at elevated temperatures. We have carried out infrared reflectivity studies of Ca_{3}Co_{2}O_{5} thin films and single crystals as a function of frequency and temperature with the emphasis on the coupling between the lattice, the charge and the spin degrees of freedom. Several important features have been observed: (1) the overall reflectivity is low as a result of a small carrier density in this system (the plasma frequency around 100 meV); (2) several phonon features are observed and some exhibit evidence of strong electron-phonon coupling; (3) a gap-like structure is seen in the low frequency region below 100 K that could be responsible to the insulating behavior observed in transport measurements at low temperatures. Further infrared studies will be performed in magnetic field (both parallel and perpendicular to the CoO2 layers). A good understanding of our infrared results should shed light on the origin of high thermo-power in these 2D-layered cobaltates.

1Supported by CUNY-RF-80209-11-13, DOE-AC02-98CH10886 and NSF-DMR-0451605.

9:24AM H43.00006 Thermoelectric properties of epitaxial Li_{2}CoO_{2} thin films. ZHIGANG MA, A. VENINADHAV, QI LI, X. X. XI, H. P. SUN, XIAOQING PAN, Penn State University — We have studied the thermoelectric properties of layered cobaltate Li_{2}CoO_{2} since the similar compound Na_{9}CoO_{2} has shown exceptionally high thermoelectric power. Both in situ epitaxial grown and topotaxial Li_{2}CoO_{2} films have been achieved. Epitaxial films were grown by pulsed-laser deposition technique and topotaxial films were prepared by converting an epitaxial CoO_{2} film to Li_{2}CoO_{2} by annealing in Li vapor. X-ray diffraction analysis showed the films are c-axis oriented. For topotaxial Li_{2}CoO_{2} the largest thermoelectric power of the samples is found to be around 380 μV/K at room temperature, while in situ films show thermopower of 100 μV/K. Both show semiconducting behaviors. The difference on the thermopower of the two types of samples will be discussed.
9:36AM H43.00007 Thermal Conductivity Minima in Superlattices and Localization-like Phenomena
RAMA VENKATASUBRAMANIAN, RTI International — It is becoming clear in many 2-dimensional superlattice (SL) material systems that there exists a minimum lattice thermal conductivity for an optimal SL period. These have been first observed and reported in the Bi$_2$Te$_3$/Sb$_2$Te$_3$/PbTe/PbTeSe and Si/Ge SL systems by us in RTI. These minima become evident when the electronic thermal conductivity, using Lorentz parameter, is subtracted from the total thermal conductivity to monitor the lattice thermal conductivity as a function of SL period. The basis for the numerical value of Lorentz parameter, observed from many facets of material and device characteristics, will be presented. Such a lattice thermal conductivity minimum has also been recently observed in other SL material systems. Recently, a similar behavior has also been observed in the thermal conductivity of superlattices embedded with an ordered array of nanoparticles. We will explore the commonality of these results in terms of a localization-like behavior for phonons. The arguments for the complex relationship between the SL period and the low-frequency cut-off wavelength, traceable to a cut-off frequency originating from diffusive transport of a temperature wave, will be presented. The physics behind what triggers the localization-like phenomena of phonons in such nanostructures will be discussed.

2DARPA/ONR Program on Thermoelectrics at RTI

9:48AM H43.00008 Si/Ge Superlattice Structures for Thermoelectric Power Generation
JAMES CAYLOR, RAMA VENKATASUBRAMANIAN, RTI International — Research conducted at RTI into the use of thin films, in particular superlattice materials, for thermoelectric power generation has focused on three materials families: Bi$_2$Te$_3$, PbTe, and Si/Ge. The Bi$_2$Te$_3$-based superlattice materials have already produced record ZT (thermoelectric figure-of-merit) and devices using these low temperature materials (~200°C) have surpassed bulk performance during power generation. RTI has also developed the growth of Si/Ge superlattice films as well as their fabrication into power generation devices applications at higher temperatures (~500°C). Results presented will include confirmation of superlattice structure via X-ray diffraction, showing well formed satellite peaks indicative of a high-quality superlattice. In addition, data will be presented that shows the lowering of thermal conductivity by the superlattice structure with nearly a 5x reduction in lattice thermal conductivity compared to the alloy film. Initial thin-film power device results showing >2% efficiency and 2x improvement of ZT over SiGe alloys, at ∆T of 378K and T$_{mean}$ of 484K, will be presented.

10:00AM H43.00009 Ultra-low thermal conductivity in disordered, layered tungsten diselenide
CATALIN CHIRIȚESCU, DAVID CAHILL, University of Illinois at Urbana-Champaign, NGUYEN NGOC, DAVID JOHNSON, University of Oregon, ARUN BODAPATI, PAWEL KEBLINSKI, Rensselaer Polytechnic Institute, PAUL ZSCHACK, Argonne National Lab — Ultra low thermal conductivity of tungsten diselenide (WSe$_2$) thin films is achieved by controlling order and disorder of two dimensional WSe$_2$ sheets. We prepared highly textured nanocrystalline WSe$_2$ films by modulated elemental reactant (MER) method. Synchrotron X-ray diffraction shows the WSe$_2$ sheets are well aligned with the Si (100) substrate and the films have completely random crystalline orientation in the a-b plane. The cross-plane thermal conductivity of thin films of WSe$_2$ is as small as 0.05 W/m-K at room temperature, 3 times smaller than the c-axis thermal conductivity of single-crystal WSe$_2$ and a factor of 6 smaller than the predicted minimum thermal conductivity for this material. Molecular dynamics simulation on model structures suggests that the ultra-low thermal conductivity in layered, disordered crystals is a general phenomenon and not restricted to WSe$_2$. Ion irradiation of the samples disrupted the layered structure and the crystallinity of the WSe$_2$ sheets and lead to an increase with a factor of 3 in thermal conductivity. We attribute the ultra-low thermal conductivity to the localization of lattice vibrations induced by the random stacking of two-dimensional crystalline WSe$_2$ sheets.

10:12AM H43.00010 Micro- and nanomachined tools for measuring in-plane thermal conductivity of thermoelectric thin films
R. RAHMAN, R. SULTAN, F. BASET, B. L. ZINK, University of Denver — Many of the potential next-generation thermoelectric materials being studied are either thin films or nanostructures that are expected to have anisotropic properties. For example, the thermal conductivity of a layered thin film in the plane of the film, $k_{\parallel}$, is likely to be different from that perpendicular to the layers, $k_{\perp}$. Techniques such as the $\Delta$ω method and picosecond thermoreflectance allow accurate measurements of $k_{\parallel}$ at temperatures relevant to thermoelectrics, but measuring $k_{\perp}$ is often difficult. In this talk we discuss our efforts to design and demonstrate accurate measurements of $k_{\perp}$ of thin films from 77 – 473 K using micro- and nanomachined thermal isolation platforms. Using thin-film structures to support the thin-film sample reduces background contributions, and careful control of the geometry keeps radiation errors small. We will also discuss plans for a next-generation device that will simultaneously measure thermal conductivity, thermopower, and electrical conductivity of a thin-film or nanostructure, allowing determination of the thermoelectric figure-of-merit, ZT.

10:24AM H43.00011 Figure of merit for thermoelectric power generation estimated from enhanced mobility in [100] oriented $\beta$-FeSi$_2$ thin film
HIROFUMI KAKEMOTO, Tokyo Institute of Technology, HAJIME SHIBATA, AIST, SATOSHI WADA, TAKA-AIKO ISHIBU, Tokyo Institute of Technology — The $\beta$-FeSi$_2$ has been attracted to be applied to the thermoelectric device, for instance, the Seebeck coefficient shows the maximum value above 500°C and it is good for thermoelectric power generation. However low figure of merit (Z) has been reported about 5x10$^{-4}$ K$^{-1}$. The Z is represented as $m^2/k_{ph}$, where $m^*$, $\mu$ and $k_{ph}$ are effective mass, mobility and thermal conductivity, respectively. Although $k_{ph}$ is good for thermoelectric power, low $\mu$ has been reported as polaronic-conduction in $\beta$-FeSi$_2$ crystal. In 3D electron density distribution of $\beta$-FeSi$_2$ crystal, Si layer in the crystal shows covalent bonding network with Si atoms, and it suggests the new possibility for enhancement of $\mu$. In this report, the objective is to discuss the possibility for enhancement of Z in order to control the crystallographic orientation of $\beta$-FeSi$_2$ crystal by means of film formation. $\beta$-FeSi$_2$ thin film was prepared on Si(100) substrate using molecular beam epitaxy method. The crystallographic orientation of sample showed about 80% of [100] direction from x-ray diffraction pattern. The transport properties were investigated using Hall measurement with van der Pauw electrode configuration. The resistivity and $\mu$ were also measured, and they were compared with $\beta$-FeSi$_2$ polycrystal. In addition, enhancement of Z was estimated using above formula.

10:36AM H43.00012 High-temperature ZT of InGaAlAs Thin Films with Embedded ErAs Nanoparticles
RAJEESH SINGH, ZHI XI BIAN, YOUNES EZZAHRI, ALI SHAKOURI, Electrical Engineering Department, University of California, Santa Cruz, GEHONG ZENG, JOHN BOWERS, Department of Electrical and Computer Engineering, University of California, Santa Barbara, JOSHUA ZIDE, ART GOSSARD, Materials Department, University of California, Santa Barbara — We have measured the thermoelectric (TE) figure-of-merit (ZT) of InGaAlAs thin films with embedded ErAs nanoparticles over a wide temperature range (300K - 650K). This material system is currently being explored for use in power generation applications such as waste heat recovery. A novel high-speed measurement system was developed to measure the ZT of thin films of thicknesses on the order of 1µm with a transient thermal signal resolution of 200ns at temperatures up to 900K. In order to resolve the intrinsic ZT of thin-film materials, TE devices were fabricated to minimize electrical and thermal parasitics and differential measurement was employed on TE devices of varying film thicknesses. The improvement in ZT of the material with ErAs nanoparticles embedded in the semiconductor matrix is verified throughout the temperature range. The increase in TE ZT is found to be mainly due to the reduction in material thermal conductivity due to phonon scattering by the ErAs nanoparticles.
Metal-Semiconductor Hybrid Systems.

acknowledge financial support of the Deutsche Forschungsgemeinschaft via the SFB 508 "Quantum Materials" and the Graduiertenkolleg 1286 "Functional...

close to the optical field maximum, are good candidates for both, new optoelectronic devices and cavity quantum electrodynamic experiments. We gratefully...

microtube as a thin dielectric waveguide forming a closed ring. These novel microtube ring resonators, in which the optically active material is intrinsically located...

running circularly around the microtube's axis inside its wall. The mode structure is in very good agreement with the result of a theoretical modeling of the...

-200 nm. We demonstrate these structure to act as optical ring resonators by measuring the photoluminescence of an optically active material, either quantum...

µm we utilize the self-rolling mechanism of strained bilayers to fabricate self-supporting microtubes with diameters of about 5...

-antibunched photon emission and can be driven into Rabi oscillations using pulsed excitation.

the quantum dot emission, coupled to the resonant cavity modes, was effectively decoupled from the excitation field. The latter was introduced via waveguide...

in a microcavity. Optics and Photonics (CREOL), University of Central Florida, W. MA, J. ZHANG, G. J. SALAMO, M. XIAO, Department of Physics, University of Arkansas, C. K. SHIH, Dept. of Physics, The University of Texas at Austin — We have studied photoluminescence upconversion in single self-assembled InGaAs quantum dots that are embedded in a planar optical microcavity. Upconversion is generally thermal and can be characterized unambiguously due to the absence of inhomogeneous broadening. A side-excitation photoluminescence technique allows us to detect arbitrarily close to the laser line thereby distinguishing otherwise unsolvable energy splittings. This allows the investigation of upconversion as a function of both temperature and energy separation.

The authors would like to acknowledge the financial support of the Canadian Institute for Photonic Innovation.

8:36AM H44.00002 Photoluminescence up-conversion of single quantum dots in a microcavity. , E. B. FLATTG, A. MULLER, X. Y. WANG, Dept. of Physics, The University of Texas at Austin, D. G. DEPPE, College of Optics and Photonics (CREOL), University of Central Florida, W. MA, J. ZHANG, G. J. SALAMO, M. XIAO, Department of Physics, University of Arkansas, C. K. SHIH, Dept. of Physics, The University of Texas at Austin — We have studied photoluminescence upconversion in single self-assembled InGaAs quantum dots that are embedded in a planar optical microcavity. Upconversion is generally thermal and can be characterized unambiguously due to the absence of inhomogeneous broadening. A side-excitation photoluminescence technique allows us to detect arbitrarily close to the laser line thereby distinguishing otherwise unsolvable energy splittings. This allows the investigation of upconversion as a function of both temperature and energy separation.

This work was supported by the National Science Foundation (grant #0604469). The authors would like to acknowledge the financial support of the Canadian Institute for Photonic Innovation.

8:48AM H44.00003 Low-threshold few-emitter quantum dot lasing. , GLENN SOLOMON, NIST Physics Laboratory, Gaithersburg, MD, WEI FANG, NIST-Physics Laboratory, Gaithersburg, MD, STEPHAN GOETZINGER, Laboratorium fur Physicalische Chemie, ETH Zurich, Zurich Switzerland, ZHIGANG XIE, Stanford University, Stanford CA — Ultra-low threshold lasing via a single emitter is of strong fundamental interest in solid-state and atomic physics. While lasing from a single emitter has not yet been observed in solid-state systems, a quantum dot (QD) gain medium gain medium of only a few QD states can be coupled to an optical cavity mode and lase. We describe such an ultra-low threshold lasing system here utilizing a microdisk cavity and a dilute QD gain medium. The microdisk is GaAs and supports high quality-factor whispering gallery modes. The QD gain medium is composed of InAs-based QDs formed epitaxially through lattice mismatch strain. Our systems show lasing even in the smallest, sub-2 micrometer disk diameters. Because of the high cavity quality factor, we observe nondegenerate modes due to broken symmetry. A typical QD spectrum of discrete emission lines observed at lower pump power is often highly modified near transparency leading to pump power dependent absorption. Changes in the cavity linewidth, second-order correlation measurements, and output emission versus input pumping are used to verify lasing. The system has sub-microwatt CW lasing thresholds and exhibits lasing from a small number of emitters.

9:00AM H44.00004 Resonance photoluminescence from a single semiconductor quantum dot in a microcavity. , A. MULLER, E.B. FLATTG, X.Y. WANG, Department of Physics, The University of Texas at Austin, D.G. DEPPE, College of Optics and Photonics (CREOL), University of Central Florida, W. MA, J. ZHANG, G.J. SALAMO, M. XIAO, Department of Physics, University of Kansas, C.K. SHIH, Department of Physics, The University of Texas at Austin — The analogue of resonance fluorescence in atomic physics is demonstrated for the first time in a zero-dimensional solid-state system consisting of self-assembled InGaAs quantum dots. The dots were embedded in a planar microcavity so that the quantum dot emission, coupled to the resonant cavity modes, was effectively decoupled from the excitation field. The latter was introduced via waveguide modes with a fiber in a side-excitation configuration. The result is a background-free detection of a single quantum dot’s photoluminescence which shows antibunched photon emission and can be driven into Rabi oscillations using pulsed excitation.

9:12AM H44.00005 Optical microtube ring resonators formed by rolled-up strained semiconductor bilayers. , TOBIAS KIPP, CHRISTIAN STRELOW, HOLGER WELSch, CHRISTIAN HEYN, DETLEF HEITMANN, Institute of Applied Physics, University of Hamburg, Germany — Starting from an epitaxially grown InGaAs/GaAs bilayer and using optical lithography and wet-etching processes, we utilize the self-rolling mechanism of strained bilayers to fabricate self-supporting microtubes with diameters of about 5 µm and wall thicknesses of only 100 - 200 nm. We demonstrate these structure to act as optical ring resonators by measuring the photoluminescence of an optically active material, either quantum wells or self-assembled quantum dots, which is embedded into the tubes’ walls. We find spectra of sharp modes arising from constructive interference of light running circularly around the microtube’s axis inside its wall. The mode structure is in very good agreement with the result of a theoretical modeling of the microtube as a thin dielectric waveguide forming a closed ring. These novel microtube ring resonators, in which the optically active material is intrinsically located close to the optical field maximum, are good candidates for both, new optoelectronic devices and cavity quantum electromagnetic experiments. We gratefully acknowledge financial support of the Deutsche Forschungsgemeinschaft via the SFB 508 “Quantum Materials” and the Graduiertenkolleg 1286 “Functional Metal-Semiconductor Hybrid Systems.”
9:24AM H44.00006 Voltage-controlled Deformation of Photonic Crystal Membranes, HUBERT J. KRENNER, Materials Department, UC Santa Barbara CA 93106, H. KIM, S. M. THON, D. BOUWMEESTER, Physics Department, UCSB, N. G. STOLTZ, P. M. PETROFF, Materials Department, UCSB — We present a novel photonic device consisting of a free-standing Photonic Crystal (PC) membrane which can be mechanically deformed by an external voltage. This is realized by introducing doped layers in the membrane and the underlying substrate. We embed self-assembled InAs quantum dots (QDs) in the membrane as active emitters. In a first step metal contacts are fabricated for both doped layers of the device. Two-dimensional PC microcavities are defined by electron beam lithography and ICP etching. The PC membrane is finalized by selectively removing an AlGaAs layer underneath the patterned region. By applying a bias voltage between the two contacts we are able to change the electrostatic force between the substrate and the membrane analogous to a plate capacitor. Due to the small thickness of the membrane the electrostatic force leads to a deformation with vertical displacements up to 250nm at room temperature. We demonstrate that at low temperatures this displacement can be reversibly changed over a wide range by an external voltage leading to a visible deformation of the membrane. We present first results of micro-PL experiments to probe the influence of the deformation on the optical modes of PC microcavities. — Supported by the Alexander-von-Humboldt Foundation

9:36AM H44.00007 Controlling the Optical Properties of Self-Assembled Quantum Dots Using External Strain, M. ZIELINSKI, NRC, Ottawa, W. JASKOLSKI, UMk, Torun Poland, G. W. BRYANT, J. DIAZ, NIST, Gaithersburg, J. AIZPURUA, DIPC, San Sebastian — Passive control of the optics of self-assembled quantum dots is achieved by controlling dot size, shape and composition via growth. Local strain from lattice mismatch between the dot and barrier influences the electronic properties. Dynamical control could be achieved via imposed external strain to change level degeneracies, polarize transitions, or modify coupling between dots. Moreover dots could be coupled to bending modes to optically cool nanomechanical oscillators to the quantum limit. To understand the impact of externally imposed strain on the electronic states of self-assembled dots, we use a tight-binding theory of dots that incorporates local strain from lattice mismatch and externally imposed strain from applied stressors or the bend in a nanomechanical oscillator. Energy level shifts depend on the position of the dot in a nanomechanical oscillator and how the oscillator is bent. Energy levels can red-shift and blue-shift depending on how the external strain is imposed. Shifts in the electronic levels due to different bending modes are determined. This allows us to assess how much active control is possible.

9:48AM H44.00008 Strong Second Order Piezoelectric Effect in InGaAs/GaAs Nanostructures, GABRIEL BESTER, ALEX ZUNGER, National Renewable Energy Laboratory, XIFAN WU, DAVID VANDERBILT, Rutgers University — We show that the piezoelectric effect that describes the emergence of an electric field in response to a crystal deformation has strong contributions in III-V semiconductors such as GaAs and InAs from second-order effects that have been neglected so far. We calculate the first and second-order piezoelectric tensors using density functional theory. Applying these calculated tensors to quantum wells [1] gives piezoelectric fields that agree well with experiments, whereas neglect of non-linearities leads to qualitative disagreements. We find that the linear and the quadratic piezoelectric coefficients have the opposite effect on the field. Which term dominates is strongly dependent on concentration x for quantum wells and for large x the quadratic terms strongly dominates. Applying our theory to quantum dots [2] shows that both terms nearly cancel each other so neglecting piezoelectricity is a better approximation than using only the linear term. Thus, the piezoelectric field turns out to be a rare example of a physical quantity for which the first-order and second-order contributions are of comparable magnitude.

10:00AM H44.00009 Single molecule fluorescence decay rate statistics in clusters of nanoparticles, LUIS FROUFE, Laboratoire EM2C, CNRS, Ecole Centrale Paris, 92295 Chatenay-Malabry, France, JUAN JOSE SAENZ, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain, REMI CARMINATI, Laboratoire EM2C, CNRS, Ecole Centrale Paris, 92295 Chatenay-Malabry, France — In this work, we study the fluorescence rate statistics of a single emitter in a finite size (nanoscopic) random medium (cluster), made of small spherical particles. For a given configuration of the system, we calculate numerically the Green tensor of the system. We deduce the spontaneous decay rate 1, as well the radiative and the nonradiative contributions. Repeating the calculation for the configuration distribution allows to compute the full statistics. These numerical experiments are used as a basis for a physical discussion. We focus on the regime in which the statistics is determined by near field interactions, with negligible multiple scattering. The decay rate statistics is influenced by the local environment of the emitter. In particular, we show that for moderate absorption, the nonradiative contribution is proportional to the imaginary part of the dielectric function of the particles, while the radiative contribution is almost constant. An important result is that the standard deviation exhibits different regimes dominated by either near-field scattering or absorption. This quantity could be used for nanoscale imaging in complex media.

10:12AM H44.00010 Diffusion limit in complex media, LEV DEYCH, Queens College of CUNY, MIKHAIL EREMETCHOUK, University of Central Florida, HUI CAO, HEESEO NOH, Northwestern University, ALEXANDER LISYANSKY, Queens College of CUNY — Structures with pre-engineered spatial modulations of the dielectric function attract a lot of attention because they provide possibility to control effectively propagation of light. Recently it has been realized that unusual optical properties of such structures have a deep impact on their general physical properties. Even such well-studied phenomena as light transport in disordered media is strongly affected by the regular modulation of the dielectric function. As a result, the transport in complex media has specific features, which can not be understood in the framework of the standard theory. We present the general theory of the diffusive (completely incoherent) limit in disordered structures with regular modulation of the dielectric function. We establish a relation between this limit and equilibrium understood from the statistical physics point of view. We show, in particular, that in the case of weak disorder the diffusion limit is virtually independent on the disorder and is nontrivially determined by properties of the ideal structure. We demonstrate how the diffusion of light appears as the perturbation of equilibrium.

10:24AM H44.00011 Aperiodic nanostructured optical devices fabricated with a femtosecond laser, TIMOTHY GERKE, JEREMY BROWN, University of Colorado at Boulder, WENJIAN CAI, KLA Tencor, ARIEL LIBERTUN, RAFAEL PIESTUN, University of Colorado at Boulder — Periodic three-dimensional (3D) structures have increasingly caught the attention of the scientific community. Aperiodic 3D structures, however, have remained relatively unexplored. We present structural and optical characterization of 3D aperiodic nanostructures created by scanning focused femtosecond (fs) laser pulses to produce permanent refractive index changes inside glass. We created polarization-sensitive devices using the effect of fs-laser-induced birefringence in fused silica. In this regime, the laser-created plasma gives origin to subwavelength structures that generate anisotropy by the effect of form birefringence. We demonstrated polarization-selective computer-generated holograms using this effect in three dimensions. These holograms form different reconstructions for different illuminating polarization states.

10:36AM H44.00012 ABSTRACT WITHDRAWN
nanoscale characterization. We will provide an overview of the challenges and opportunities in these areas and describe how advances here could impact heterogeneous nanostructures, innovative photon management, enhanced light-matter interactions, multiscale modeling for solid-state lighting, and precise research areas that have potential to impact solid-state lighting. Basic research in the following areas were identified as priorities: new functionality through polyfluorenes. We then shift our attention to charge injection. We review some of the recent theories and compared their predictions to experimental data, for the influence of disorder on mobility, for high charge densities, and for electric field-dependent charge densities. We compare with experimental data from Brookhaven National Lab — The recent DOE workshop on basic research needs for solid-state lighting has identified a number of cross-cutting scientific limitations of experimental techniques that are used to probe charge transport. We then embark on a discussion of the fundamentals of charge transport in Cornell University — We will overview the state-of-the-art in our understanding of charge injection and transport in conjugated polymers. We start by discussing the identifying characteristics of this class of materials, especially in relation with their structure and morphology. We follow by reviewing the advantages and limitations of experimental techniques that are used to probe charge transport. We then embark on a discussion of the fundamentals of charge transport in organics. We follow a didactic approach, where we start from transport in crystalline semiconductors and gradually introduce corrections for space charge effects, for the influence of disorder on mobility, for high charge densities, and for electric field-dependent charge densities. We compare with experimental data from polyfluorenes. We then shift our attention to charge injection. We review some of the recent theories and compared their predictions to experimental data, again from polyfluorenes. We close by proposing directions for future work.


11:15AM J3.00001 Current State of the Art in High Brightness LEDs , GEORGE CRAFORD, Philips Lumileds Lighting Company — LED’s have been commercially available since the 1960’s. For many years they were used primarily for indicator applications. The remarkable increase in materials technology and efficiency that has been achieved since the early 1990’s for AlInGaP red and amber LEDs, and InGaN green and blue LEDs, has enabled the penetration of markets such as outdoor display, signaling, and automotive brake light and turn signal applications. White LEDs, which are either blue LEDs combined with a phosphor, or a combination of red, green, and blue LEDs, are being used in emerging applications such as cell phone flash, television backlights, projection, and automotive headlights. In addition, to efficiency improvements these applications have required the development of higher power packages and, in some of these applications which are etendue limited, higher luminance devices. High power devices are commercially available which are capable of 140 lumens output and have an efficacy of around 70 lm/W for white emission. New package and chip technologies have been demonstrated which have a luminance of 38 mega nits (Mcd/m²), approximately 50% more luminance than that of an automotive headlamp halogen bulb (~25 mega nits). The recent progress in materials technology, packaging, and chip technology makes it clear that LED’s will become important for general illumination applications. The rate of LED penetration of this market will depend upon continued increases in performance and lower costs as well as better control of the white spectral emission. Efficiency, current density, and costs are closely linked because the cost in dollars/lumen is inversely proportional to how many lumens can be realized from each unit of device area for a given device type. Performance as high as 138 lm/W, and over 40% wall plug efficiency, has been reported for low power research devices and over 90 lm/W for high power research devices. It is clear that high power commercial products with performance in excess of 100 lm/W will become available soon, which is substantially more efficient than incandescents (~15 lm/W) and compact fluorescents (~60 lm/W) and equivalent to high performance fluorescent lighting. Performance in the range of 150 lm/W or even higher is plausible in the longer term. This talk will include an overview of the status and trends in LED technology and applications, and the challenges which must be met in order for LED’s to become widely utilized in general illumination.


1:03PM J3.00004 Charge Injection and Transport in Conjugated Polymers . , GEORGE MALLIASARAS, Cornell University — We will overview the state-of-the-art in our understanding of charge injection and transport in conjugated polymers. We start by discussing the identifying characteristics of this class of materials, especially in relation with their structure and morphology. We follow by reviewing the advantages and limitations of experimental techniques that are used to probe charge transport. We then embark on a discussion of the fundamentals of charge transport in organics. We follow a didactic approach, where we start from transport in crystalline semiconductors and gradually introduce corrections for space charge effects, for the influence of disorder on mobility, for high charge densities, and for electric field-dependent charge densities. We compare with experimental data from polyfluorenes. We then shift our attention to charge injection. We review some of the recent theories and compared their predictions to experimental data, again from polyfluorenes. We close by proposing directions for future work.

1:39PM J3.00005 Cross-Cutting Basic Research Needs for Solid State Lighting¹ , JAMES MISEWICH, Brookhaven National Lab — The recent DOE workshop on basic research needs for solid-state lighting has identified a number of cross-cutting scientific research areas that have potential to impact solid-state lighting. Basic research in the following areas were identified as priorities: new functionality through heterogeneous nanostructures, innovative photon management, enhanced light-matter interactions, multiscale modeling for solid-state lighting, and precise nanoscale characterization. We will provide an overview of the challenges and opportunities in these areas and describe how advances here could impact solid-state lighting.

¹This work was supported by the DOE Office of Basic Energy Sciences

Tuesday, March 6, 2007 11:15AM - 2:03PM – Session J8 DMP: Focus Session: Novel Superconductors IV: Intercalated graphites and related Colorado Convention Center Korbel 1C
11:15AM J8.00001 Superconductivity in alkaline earth-intercalated graphites: CaC$_6$ and SrC$_6$$^1$

JUN SUNG KIM, Max-Planck-Institut fuer Festkoerperforschung — The recent discovery of superconductivity in alkaline earth-intercalated graphites CaC$_6$ ($T_c = 11.5$ K) with substantially higher $T_c$’s than the previously known, has renewed the interest in the graphite intercalated compounds and stimulated a debate about the relevant pairing mechanisms. We have investigated the superconducting properties of high-quality CaC$_6$ samples, using specific heat ($C_P$) and magnetization measurements. For CaC$_6$, the exponential temperature dependence of the electronic $C_P$ and its linear dependence on the magnetic fields provide evidence for a fully-gapped, intermediate-coupled, and phonon-mediated superconductor without essential contributions from alternative pairing mechanisms. However, the $C_P$ anomaly at $T_c$ is found to be much smaller than expected from theory, indicating a possible anisotropy in the superconducting gap. Consistently, the anisotropy of the upper critical field $H_{c2}^u/H_{c2}^l$ is also larger than expected from the Fermi velocities, and shows significant temperature dependence below $T_c$. Recently, we also discovered the superconductivity in SrC$_6$ at $T_c = 1.65(6)$ K as well as the absence of superconductivity in BaC$_6$ down to 0.3 K. Similar to CaC$_6$, the $C_P$ anomaly of SrC$_6$ is somewhat lower than that theory predicted, but the discrepancy is much reduced. The anisotropy of $H_{c2}$ for SrC$_6$ is also found to be much smaller than that of CaC$_6$, indicating a reduced superconducting gap anisotropy. Finally, we will discuss the significantly lower $T_c$ of SrC$_6$ than CaC$_6$ as well as their positive pressure dependence in terms of the $e$-$ph$ coupling with the in-plane intercalant and the out-of-plane C phonon modes, based on ab-initio calculations. Implications of the present findings on the superconducting mechanisms in alkaline-earth as well as alkalii-intercalated graphites will also be given.


---

11:51AM J8.00002 Bulk evidence for single-gap s-wave superconductivity in the intercalated graphite superconductor Ca$_6$Yb

NICOLAS DORION-LEYRAUD, Universite de Sherbrooke and CIAR, THOMAS WELLER, MARK ELLERBY, University College London, MONTU SAXENA, University of Cambridge — We report measurements of the in-plane electrical resistivity $\rho$ and thermal conductivity $\kappa$ of the intercalated graphite superconductor Ca$_6$Yb to temperatures as low as $T_c$. When a magnetic field is applied along the c-axis, the part of $\kappa$ associated with fermionic quasiparticles increases exponentially for $H_x < H < H_{c2}/2$. This activated behaviour is consistent with an s-wave order parameter, as well as being strong evidence against a multi-gap scenario.

---

12:03PM J8.00003 Superconductivity in Alkali-Earth intercalated graphite.

MATTEO CALANDRA, FRANCESCO MAURI, IMPMC, Universite de Paris 6 — It has long been known that Graphite intercalated compounds (GICs) can display a superconducting behavior at low temperature. However, until the discovery of YbC$_6$ and CaC$_6$, the critical temperatures achieved were typically inferior to 5 Kelvin. Using density functional theory we study superconductivity in AC$_6$ with A=K, Rb, Sr, Ca, Ba and Mg$_{1-x}$Ca$_x$. We find that at zero pressure Ca, Ba and Sr intercalated graphite are superconducting with critical temperatures ($T_c$) 11.5 K, 0.2 K and 3.0 K, respectively. We study the pressure dependence of $T_c$. We find that the SrC$_6$ and BaC$_6$ critical temperatures should be substantially enhanced by pressure. On the contrary, for CaC$_6$ we find that in the 0 to 5 GPa region, $T_c$ weakly increases with pressure. The increase is much smaller than what shown in several recent experiments. Thus we suggest that in CaC$_6$ stacking faults or a continuous phase transformation, such as an increase in staging could occur at finite pressure. Finally we argue that Mg$_{1-x}$Ca$_x$C$_6$ could lead to higher critical temperatures.

---

12:15PM J8.00004 Far-infrared signature of a superconducting gap in intercalated graphite CaC$_6$

U. NAGEL, D. HUVONEN, T. ROOM, NICPB, Tallinn, J.S. KIM, L. BOERI, R. K. KREMER, MPI for Solid State Physics, Stuttgart, F. S. RAZAVI, Brock Univ., St. Catharines, Ont. — CaC$_6$ is exceptional in the series of intercalated graphite compounds because of its high superconducting transition temperature, $T_c$=11.5K. The superconducting gap, $2\Delta$=25.6 ± 3.2 cm$^{-1}$, measured by scanning tunneling spectroscopy (N. Bergeal et al., PRL 97, 070703 (2006)), is consistent with the weak-coupling BCS type superconductivity. The superconducting gap can be directly probed also by far-infrared spectroscopy. We studied the reflectance $R$ of CaC$_6$ between 4 and 100cm$^{-1}$ from 3K to 15K. We see the signature of the superconducting gap in the reflectance ratio of superconducting state $R_s$ to the normal state $R_n$ and can follow its temperature dependence. The appearance of the gap signature in $R_s/R_n$ tells us that CaC$_6$ is in the dirty limit. Different models, including an anisotropic gap and a multi-gap scenario, will be discussed to fit the optical data.

---

12:27PM J8.00005 A First-Principles Insight into the Superconductivity of Graphite Intercalation Compounds

LILIA BOERI, OLE KROGH ANDERSEN, JUN SUNG KIM, REINHARD KREMER, Max-Planck-Institut fuer FestkoerperForschung, Stuttgart, Germany, MATTEO GIANTOMASSI, U.P.C.M., Universite Catholique de Louvain, Louvain-la-Neuve, Belgium, GIOVANNI B. BACHELET, INFM SMC and Dipartimento di Fisica, Universita la Sapienza, Roma, Italy, FERIDON S. RAZAVI, Department of Physics, Brock University, Ontario, Canada — Experimental evidence has established that the recently discovered superconductivity in graphite-intercalation compounds (GICs) CaC$_6$ and YbC$_6$ is due to electron-phonon ($e - ph$) coupling. First-principles calculations predict for CaC$_6$ an intermediate $e - ph$ coupling ($\lambda \approx 0.8$), resulting from intercalant in-plane ($I_{xy}$) and carbon out-of-plane ($C_{z}$) vibrations. Whereas the softening of the $I_{xy}$ modes explains increase of $T_c$ with pressure [1], the presence of the $C_z$ peak is due to an interaction which is “dormant” in pure graphite. A simple analysis of the band structure of the GICs also permits to rule out the possibility of plasmon-mediated superconductivity[1].


---

12:39PM J8.00006 Strong electron-phonon coupling in the rare-earth carbide superconductor La$_2$C$_3$

REINHARD K. KREMER, J.S. KIM, W.-H. XIE, V. BABIZHETSKYY, O. JEPSEN, A. SIMON, MPI fuer FestkoerperForschung, Stuttgart, Germany, K.S. AHN, B. RAQUET, Yonsei University, Wonju, South Korea, H. RAKOTO, J.-M. BROTO, LNCMP, Toulouse, France, B. OULADDIAF, ILL, Grenoble, France — Superconductivity in rare earth carbides has attracted interest again after the recent discovery of the 18 K superconductor Y$_2$C$_3$. Here, we present the crystal structure as well as the superconducting properties of the rare-earth sesquicarbides La$_2$C$_3$ ($T_c \approx 13.4$ K) gained from low-temperature neutron powder diffraction, specific heat and electrical resistivity measurements. From a detailed analysis of specific heat as well as the comparison with the full potential electronic structure calculations, a first-principles estimate of the electron-phonon coupling strength and the logarithmic average phonon frequency is made. The electron-phonon coupling constant found to be $\lambda_{ph} \sim 1.35$, and the low energy phonon modes are responsible for the superconductivity. These results suggest that La$_2$C$_3$ is in the strong coupling regime and the relevant phonon modes are the La-related modes rather than the C-C stretching modes. The upper critical fields ($H_{c2}$) show a clear enhancement with respect to the Werthamer-Helfand-Hohenberg prediction and amount to $H_{c2}(0) \approx 20$ T confirming the strong electron-phonon coupling.
12:51PM J8.00007 The potential for mean-field d-wave superconductivity in graphite, ANNICA BLACK-SCHAFFER, Stanford University, SEBASTIAN DONIACH — We investigate the possibility of inducing superconductivity in a graphite layer by electronic correlation effects. We use a phenomenological microscopic Hamiltonian [1] which includes nearest neighbor hopping and an interaction term which explicitly favors nearest neighbor spin-singlets through the well-known resonance valence bond (RVB) character of planar organic molecules. Treating the Hamiltonian in mean-field theory, allowing for bond-dependent variation of the RVB order parameter, we show that both s- and d-wave superconducting states are possible with the d-wave state having a significantly higher $T_c$ at finite doping. By using density functional theory we show that the doping induced from sulfur absorption on a graphite layer is enough to cause an electronically driven d-wave superconductivity at graphite-sulfur interfaces (see e.g. [2]). We will also briefly discuss applying our results in the case of the intercalated graphitees as well as the validity of a mean-field approach.


1:03PM J8.00008 Possibility of superconductivity in high pressure phases of BC$_3^{1}$, JONATHAN E. MOUSSA, MARVIN L. COHEN, UC Berkeley & LBNL — Using an ab-initio pseudopotential-local-density-approximation, we study the possibility of a high-pressure transition of graphitic planar sp$^2$ bonded BC$_3$ into an sp$^3$ bonded covalent network. Energy barriers are examined for the predicted transition to the sp$^3$ phase and for the observed onset of phase separation in BC$_3$ under high pressure, high temperature conditions [V. L. Solozhenko et al., Appl. Phys. Lett. 85, 1508 (2004)]. The sp$^3$ phase of BC$_3$ is predicted to be metallic and superconducting and is similar to 25% boron-doped diamond without boron clusters. Calculations of phonon frequencies and electron-phonon coupling allow for an estimate of the superconducting transition temperature.

$^1$This work was supported by National Science Foundation Grant No. DMR04-39768, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC.

1:15PM J8.00009 Probing electronic structure and electron-phonon interaction in borides using optical spectroscopy, JEREMIE TEYSSIER, ALEXEY KUZENKO, RICCARDO TEDIOSI, DIRK VAN DER MAREL, DPMC, University of Geneva, 1211 Geneva 4, Switzerland, NATALIA SHITSEVALOVA, VLADIMIR FILIPPOV, IPMS, Academy of Sciences of Ukraine, 252680 Kiev, Ukraine — We report optical properties of high-quality single crystals of boron type superconductor ZrB$_2$. The optical conductivity was measured from (6 meV-4 eV) by a combination of reflectivity and ellipsometry. The Drude plasma frequency and interband optical conductivity calculated by self-consistent full-potential LMTO method agree well with experiments. The $\alpha(T)$ function extracted from optical spectra presents two peaks at 25 and 80 meV with partial coupling constants of 0.8 and 0.3 respectively. The low energy peak corresponds to the displacement of Zr inside B$_2$ cages, while the second one involves the rigid LMTO network. In addition to the usual narrowning of the Drude peak with cooling down, we observed an unexpected removal of about 10% of the Drude spectral weight which is partially transferred to the region of the lowest-energy interband transition ($\approx 1$ eV). This effect may be caused by a delocalization of the metal ion from the centre of the B$_2$ cage. The discussion will refer to recent work on other boron rich compounds.

1:27PM J8.00010 Gapless Fermi Surfaces in anisotropic multiband superconductors in magnetic field., VICTOR BARZYKIN, Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, LEV P. GOR’KOV, National High Magnetic Field Laboratory, Florida State University, 1800 E. Paul Dirac Dr., Tallahassee, Florida 32310 — We propose that a new state with a fully gapless Fermi surface appears in quasi-2D multiband superconductors in magnetic field applied parallel to the plane. It is characterized by a paramagnetic moment caused by a finite density of states on the open Fermi surface. We calculate thermodynamic and magnetic properties of the gapless state for both s-wave and d-wave cases, and discuss the details of the 1-st order metamagnetic phase transition that accompanies the appearance of the new phase in s-wave superconductors. We suggest possible experiments to detect this state both in the s-wave (2-H NbSe$_2$) and d-wave (CeCoIn$_5$) superconductors.

$^1$This work was supported (VB) at the University of Tennessee and (LPG) by NHFML through the NSF Cooperative agreement No. DMR-008473 and the State of Florida.

$^2$Also at L.D. Landau Institute for Theoretical Physics, Chernogolovka, 142432, Russia

1:39PM J8.00011 Superconducting order parameter in NbSe$_2$ derived from the specific heat, JIUNN-YUAN LIN, H. Y. SHEN, Institute of Physics, National Chiao-Tung University, Hsinchu 300, Taiwan, H. D. YANG, C. L. HUANG, C. P. SUN, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, T. K. LEE, Institute of Physics, Academia Sinica, Nankang 11592, Taiwan, H. BERGER, Institute of Physics of Complex Matter, EPFL, Lausanne, Switzerland — To resolve the discrepancies on the superconducting order parameter of quasi-2D NbSe$_2$, the comprehensive specific heat measurements have been carried out. The thermodynamic consistence requires more than one energy scale of the order parameters. The zero field data and the results of the mixed states respectively with $H \parallel c$ and $H \perp c$ conclude: (1) $\Delta_s = 1.26$ meV and $\Delta_d = 0.73$ meV. (2) $N(0)/N(0) = 11\% \sim 20\%$. (3) $\Delta_s$ is 3-D and like on the Se derived Fermi surface. This present scenario largely removes the dispute over the order parameter existing in the previous literature. The alternative anisotropics-s-wave model is also discussed.

$^1$This work was supported by NSC and MOE-TAU of Taiwan

1:51PM J8.00012 Unconventional Superconductivity and Mott Transition of Expanded A3C60 Alkali Fullerides, E. TOSATTI, SISSA/ICTP/Democritos, Trieste, Italy, M. CAPONE, INFN/SMC, Rome, I-00185 Italy, M. FABRIZIO, SISSA/ICTP/Democritos, Trieste, Italy, C. CASTELLANI, Rome University La Sapienza, Italy — Although phonon-driven and s-wave, superconductivity in trivalent alkali fullerides A3C60 exhibits several unconventional features. Beyond a certain limit, a volume expansion provokes first a decrease of $T_c$, and then a superconductor-Mott insulator transition, indicating strong electron correlations. Using Dynamical Mean Field Theory (DMFT) we solved a narrow 3-band Hubbard model, including several other important on-site couplings beyond the Hubbard repulsion $U$. Mimicking expansion as an increasing $U$, the model turns from a nonsuperconducting metal, to a BCS-like superconductor with increasing gap, to a pseudogap superconductor with decreasing gap, and finally to a $s=1/2$ antiferromagnetic Mott Insulator. The last two regimes assimilate the expanded A3C60 superconductors to underdoped high $T_c$ cuprates and to 2D organic superconductors, seen as members at large of a large family. Newer experimental predictions are made.

$^1$Supported by FIRB RBAP017S8 R004, RBAU01LX5H, COFIN2004

Tuesday, March 6, 2007 11:15AM - 2:15PM –
Session J9 DMP: Superconductivity: Oxide Photoemission I and X-ray Scattering Colorado Convention Center Korbel 1D
11:15AM J9.00001 A Proposed New Measurement of the Superconducting Gap in YBa$_2$Cu$_3$O$_7$ - G.L. ZHAO, D. BAGAYOKO, Southern University and A & M College — The superconducting energy gap of YBa$_2$Cu$_3$O$_7$ (YBCO) varies strongly with field from a sheet of the Fermi surface to another. The strong anisotropic superconducting gap in high Tc materials such as YBCO has led to conflicting d-wave and s-wave interpretations. We have utilized electronic wave functions from the ab-initio density functional calculation and the related electron-phonon interaction matrix elements for the calculation of the superconducting gap values of YBCO. For three pieces of the Fermi surfaces, the calculated superconducting gaps exhibit a strong anisotropy. In contrast, we have found that the superconducting gap on one sheet of the Fermi surface around S-point only shows a minor variation from about 18 meV to 25 meV. This work was funded in part by NSF (Award No. 0508245) and ONR (Grant No: N00014-05-1-0009).

11:27AM J9.00002 Dynamic Response Functions from Angle Resolved Photoemission Spectra - UTPAL CHATTERJEE, DIRK MORR, University of Illinois at Chicago, MIKE NORMAN, Argonne National Laboratory, MOHIT RANDERIA, Ohio State University, JUAN CARLOS CAMPUZANO, University Of Illinois at Chicago — The linear response to an external probe as a function of energy and momentum is of great importance in elucidating the properties of complex materials. We introduce a formalism in the framework of diagrammatic k space approach with Random Phase Approximation (RPA), for calculating dynamic response functions using experimental single particle Green’s function derived from ARPES spectra. Specifically we focus on using the single particle Green’s function obtained from superconducting state of ARPES data in the high Tc cuprates to compute the dynamic spin susceptibility. We find good agreement between our results and the superconducting state neutron results, in particular the resonance at antiferromagnetic ordering wave vector, with its unusual ‘reverse magnon’ dispersion. We anticipate, our formalism will also be useful in interpreting results from other spectroscopies such as optical and Raman responses.

11:39AM J9.00003 Self Energy Analysis of Photoemission spectral function from parent cuprates, Ca$_2$CuO$_2$Cl$_2$ - CHUL KIM, DONG JOON SONG, CHOON SHIK LEEM, HYEONG UK JIN, SEUNG RYONG PARK, Yonsei University, HYEONG DO KIM, Pohang Accelerator Laboratory, FILIP RONNING, Los Alamos National Laboratory, CHANG YOUNG KIM, Yonsei University, YONSEI UNIVERSITY TEAM, POHANG ACCELERATOR LABORATORY COLLABORATION, LOS ALAMOS NATIONAL LABORATORY COLLABORATION — Self energy $\Sigma(k,\omega)$ is the fundamental function that describes the effects of many-body interactions on an electron in a solid. But it is very difficult to extract the self energy from experimental data, especially for non-metallic materials. In this paper we developed a new and general method with which one can extract the self energy from angle-resolved photoemission spectroscopy (ARPES) data in the full k-ω space. We demonstrate the validity of this method by applying it to the ARPES data from Ca$_2$CuO$_2$Cl$_2$ (CCOC). We find the values for the imaginary part of the self energy is compatible with the value obtained by measuring the peak width.

11:51AM J9.00004 The hierarchy of multiple many-body interaction scales in high-temperature superconductors - W. MEEVASANA, X.J. ZHOU, Z.-X. SHEN, Stanford University, S. SAHRARKORPI, A. BANSIL, Northeastern University, T. YOSHIDA, A. FUJIMORI, University of Tokyo, Kashiwa, Japan, Y. ANDO, Central Research Institute of Electric Power Industry, Japan, F. ZHOU, Z.X. ZHAO, Chinese Academy of Sciences, China, T. SASAGAWA, K. FUJITA, University of Tokyo, B. Joyo-ku, Japan, H. EISAKI, AIST, Tsukuba, Japan — Many-body interaction is key to novel properties of quantum matter. As an extreme example, the complexity due to charge, spin, and lattice interactions in high-Tc superconductors makes it difficult to identify the essential microscopic ingredients for the basic model. Energy scales where these interactions are manifest usually provide important insights into the nature of the interactions. The momentum dispersion relationship measured by angle-resolved photoemission spectroscopy (ARPES) provides an excellent tool for identifying these scales. To date, the focus of the discussion has been on the low energy anomaly near 0.03-0.09eV. Here we present improved experimental photoemission spectra from four families of high-Tc superconductors that reveal a hierarchy of many-body interaction scales on: the low energy anomaly (“kink”) of 0.03-0.09eV, a high energy anomaly of 0.3-0.5eV, and an anomalous enhancement of the width of the LDA-based CuO$_2$ band extending to energies of approximately 2 eV.

12:03PM J9.00005 Energy scales revealed by ARPES study on four layered cuprate superconductor Ba$_2$Ca$_3$Cu$_4$O$_{8-\delta}$ - YULIN CHEN, Stanford University, AKIRA IYO, AIST, Japan, WANLI YANG, XINGJIANG ZOU, WEISHENG LEE, WORAWAT MEEVASANA, DONGHUI LU, Stanford University, HIROSHI EISAKI, AIST, Japan, OLE ANDERSEN, Max-Plank Institute, Germany, THOMAS DEVEREAUX, University of Waterloo, Canada, ZAHID HUSSAIN, Advanced Light Source, LBNL, ZHI-XUN SHEN, Stanford University, ZHI-XUN SHEN TEAM, AKIRA IYO COLLABORATION, OLE K. ANDERSEN COLLABORATION, THOMAS P. DEVEREAUX COLLABORATION, ZAHID HUSSAIN COLLABORATION — Recently discovered four layered cuprate superconductor Ba$_2$Ca$_3$Cu$_4$O$_{8-\delta}$ possesses various properties that differ from the conventional high Tc superconductors, making itself exceptional to the well known high Tc superconductivity phase diagram. The understanding of this discrepancy will provide important implications for high Tc theory. We study this material by Angular Resolved Photoemission Spectroscopy (ARPES) and find that the electronic band structure of this four layered system exhibits clear difference from the previously studied hole- or electron- doped cuprate superconductors such as Bi2212 or NCCO. The multiple energy scales associated with its electronic structures not only show the complexity of this system, but also provide hints to understand its uniqueness.

12:15PM J9.00006 The evolution of electronic structure of Bi$_2$Sr$_2$-xBi$_x$CuO$_6$+$\delta$ revealed by ARPES - ZHIHUI PAN, P. BISHAY, P. RICHARD, M. NEUPANE, Z. WANG, H. DING, Boston College, H.-H WEN, Institute of Physics and National Lab for Condensed Matter Physics China — Bi$_2$Sr$_2$-xLn$_x$CuO$_6$+$\delta$ (Ln is a trivalent element) is a good candidate to investigate the effects of charge doping and potential disorder to the properties of the high-Tc cuprates. High-quality single crystals of Bi$_2$Sr$_2$-xBi$_x$CuO$_6$+$\delta$ (Bi-Bi2201) have been synthesized over a wide substitution range (0 < x < 0.1) where the sample evolves from an overdoped superconductor to an insulator. We will report our ARPES results on the evolution of electronic structure of Bi-Bi2201.

12:27PM J9.00007 High-energy kink in high-temperature superconductors - PETER JOHNSON, TONICA VALLA, TIM KIDD, W.G. YIN, GENDA GU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, Z.-H PAN, ALEXEI FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, — Photoemission studies show the presence of a high energy anomaly in the observed band dispersion for two families of cuprate superconductors, Bi$_2$Sr$_2$Ca$_x$Cu$_{2-y}$O$_{6-\delta}$ and La$_2$-Ba$_x$Cu$_2$O$_y$. The anomaly, which occurs at a binding energy of approximately 340 meV, is found to be doping and momentum independent. The magnitude of the effect is momentum dependent. Scattering from short range or nearest neighbour spin excitations is found to supply an adequate description of the observed phenomena.

12:39PM J9.00008 Systematic ARPES study of n-doped cuprate superconductors - PIERRE RICHARD, MADHAB NEUPANE, YI-MING XU, PHILIPATER BISHAY, Boston College, PATRICK FOURNIER, Universite de Sherbrooke, SHILIANG LI, PENGCHENG DAI, University of Tennessee at Knoxville, ZIQUIANG WANG, HONG DONG, Boston College — In contrast to the hole-doped high-temperature superconductors, for which the Cu$_2+$ long-range antiferromagnetism (AF) is suppressed at low doping, the AF order is more robust and extends to higher doping in the case of the electron-doped superconductors RE$_2$-xCexCuO$_4$ (RE = Pr, Nd, Sm) and (Pr$_{1-x}$La$_x$)$_2$-xCexCuO$_4$. Even though this long-range ordering is suppressed at optimal doping, neutron measurements and Hubbard model calculations suggest the persistence of short-range fluctuations. In order to investigate the impact of these fluctuations on the electronic structure of the electron-doped superconductors, we have performed systematic angular resolved photoemission spectroscopy measurements of optimally doped Pr$_2$-xCexCuO$_4$ and (Pr$_{1-x}$La$_x$)$_2$-xCexCuO$_4$ samples. We present and discuss our recent results.

12:51PM J9.00009 s-wave-like excitation in the superconducting state of electron-doped cuprates with d-wave pairing . QINGSHAN YUAN, XIN-ZHONG YAN, CHIN-SEN TING, Texas Center for Superconductivity, University of Houston, Houston, TX 77204 — It has been quite controversial whether the superconducting (SC) pairing symmetry is s- or d-wave in electron-doped cuprates such as Nd$_{2-x}$Ce$_x$CuO$_4$ (NCCO) and Pr$_{2-x}$Ce$_x$CuO$_4$ (PCCO). In view that many experimental measurements to study the SC pairing symmetry only give direct information about the quasiparticle excitation gap and not the SC order parameter, we explore a physical mechanism to show the s-wave-like quasiparticle excitation under the d-wave SC pairing in electron-doped cuprates and intend to reconcile the contradictory experimental results. Our idea is based on the intrinsic Fermi surface (FS) evolution with doping as revealed by ARPES measurements on NCCO. It was found that at low doping only a small FS pocket appears around ($\pi$, 0) and with increasing doping a new FS pocket around ($\pi$/2, $\pi$/2) will emerge. We argue that the FS pocket around ($\pi$/2, $\pi$/2) has not yet formed during doping, but is located inside the FS pocket around ($\pi$, 0). Therefore, in the underdoped regime, even if the SC order parameter is d-wave which vanishes along the diagonal line, the quasiparticle excitation gap is still finite and looks s-wave-like due to the absence of the FS across that line. This makes it possible, with d-wave SC pairing, to understand those experiments which evidenced the s-wave quasiparticle excitation.

1:03PM J9.00010 Spectral function analysis of an e-doped Hi-Tc superconductor near optimal doping, revisited , FELIX SCHMITT, WEI-SHENG LEE, DONG HUI LU, WORAWAT MEEVASANA, EUGENE MOTOYAMA, MARTIN GREVEN, ZHI-XUN SHEN, Departments of Physics, Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, California 94305 — By comparison with the p-doped high transition temperature superconductors, their e-doped counterparts might give further insight into the unusual underlying physics. High resolution angle-resolved photoemission spectroscopy (ARPES) data of an e-doped cuprate near optimal doping is presented to further enrich previous comprehensive work on the subject. Spectral function analysis is also used to discuss band renormalizations. Other findings will be discussed as well.

1:15PM J9.00011 Intermediate energy structure of cuprates using Resonant Inelastic X-ray Scattering, JASON HANCOCK, GUILLAUME CHABOT COUTURE, LI LU, MARTIN GREVEN, KENJI ISHII, JUN’ICHIRO MIZUKI, Stanford, THOMAS GOG, DIEGO CASA, Argonne — We present a comprehensive study of the charge-transfer excitations in the 1-8 eV range using the burgeoning technique of resonant inelastic X-ray scattering (RIXS). Surprisingly, we find that the charge-transfer gap, distinct around 2.5 eV in Mott insulating La$_2$CuO$_4$, is still discernible in the high-Tc superconductor HgBa$_2$CuO$_4$. In addition, we are able to identify many distinct, weakly dispersive features above the charge-transfer gap of La$_2$CuO$_4$ [1] and the model high-Tc superconductor HgBa$_2$CuO$_{4+\delta}$ [1]. Detailed extension of this work in La$_2$CuO$_4$ reveals previously unresolved systematics in the vicinity of the charge-transfer gap, and a distinct dependence on scattering geometry of both the charge-transfer gap and the high-energy excitations. We interpret this scattering-geometry dependence as arising from the intrinsic symmetry selectivity of the RIXS/Raman process, and suggest that similar experiments can give definitive identification of excitation symmetry. [1] L. Lu et al., Phys. Rev. Lett. 95, 217003 (2005). [2] L. Lu et al. (to appear Phys. Rev. B 74; cond-mat/0607311) [3] N. J. Hancock et al. (in preparation).

1:27PM J9.00012 ABSTRACT WITHDRAWn —

1:39PM J9.00013 RIXS Spectra for Ladder Cuprate $Sr_{14}Cu_{24}O_{41}$ , W.M. AL-SAWAI, R.S. MARKIEWICZ, A. BANSIL, Northeastern University, Boston, MA 02115, L. WARRY, D. QIAN, M.Z. HASSAN, Department of Physics, Joseph Henry Laboratories, Princeton University, Princeton, NJ 08544 — The ladder compound $Sr_{14}Cu_{24}O_{41}$ is of interest both as a quasi-one-dimensional analog of superconducting cuprates and as a superconductor in its own right when $Sr$ is substituted by $Ca$. In order to model recent resonant inelastic x-ray scattering (RIXS) spectra of this compound, we studied the simpler $SrCu_2O_3$ system in which the crystal structure contains very similar ladder planes. We approximated the LDA dispersion of $SrCu_2O_3$ by two different tight-binding models - either a copper only model with two bands or a copper plus planar oxygen model with seven bands. Due to the glide symmetry of the structure, the period of dispersion along the ladder is 4\times. Strong correlation effects were treated by assuming an anti-ferromagnetic ground state for both models. The resulting dispersion of the filled band at half filling matches the experimental ARPES spectra, and the RIXS spectra are in good agreement with experimental results. Work supported in part by the USDOE.

1:51PM J9.00014 Inelastic X-ray scattering study of the bond stretching phonon mode in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, D. SIEGEL, University of California Berkeley, J. GRAF, LBNL, M. D’ASTUTO, IMPMC, A.Q.R. BARON, SPRING-8, H. EISAKI, AIST, A. LANZARA, University of California Berkeley — The phonon dispersions of the single layer high temperature superconductor $Sr_{2-x}Cu_xO_3$ along the [0 0 1] direction have been determined by inelastic x-ray scattering. The two highest longitudinal phonon branches, associated with the Cu-O bond stretching and out-of-plane oxygen vibration, are clearly resolved for the first time. The comparison with $La_{2-x}Sr_xCuO_4$ will be discussed.

2:03PM J9.00015 Structures and properties of Ni$_{1+2x}$ nickelates with infinite NiO$_2$ layers, KONSTANTIN LOKSHIN, TAKESHI EGAMI, University of Pennsylvania, VIKTOR POLTAVETS, MARTHA GREENBLATT, Rutgers University — Layered mixed valence Ni$_{1+2x}$ nickelates possess similar crystal and electronic structures to Cu$_{2+3x}$ high temperature superconducting cuprates. Only a few Ni$_{1+2x}$ nickelates have been identified and they properties have not been reported so far. We present a first systematic study of $Ln_{n+1}NiO_{2n+2}$, $Ln = La$ or Nd, which structures could be described as an intergrowth of (LnO$_x$) fluorite and infinite layer (LaNiO$_x$)$_n$ blocks. The crystal structures of the new Ln$_nNiO_8$, Ln$_nNiO_{12}$, Ln$_nNiO_{16}$ phases have been confirmed by X-ray and neutron powder diffraction. X-ray absorption spectroscopy data proves the 1+/2+ oxidation state and planar coordination of Ni atoms. Magnetic susceptibility data of $Ln_{n+1}NiO_{2n+2}$ will be discussed.

Tuesday, March 6, 2007 11:15AM - 2:15PM — Session J11 DMP: Correlated Organic Conductors Colorado Convention Center Korbel 1F

11:15AM J11.00001 Mixed spin-charge solitons and thermodynamics of (TMTTF)$_2$X , SUMIT MAZUMDAR, University of Arizona, R. TORSTEN CLAY, R. P. HARDIKAR, Mississippi State University — The (TMTTF)$_2$X salts are quasi-one-dimensional materials that undergo two phase transitions as the temperature is lowered from 300 K under ambient pressure. The high temperature transition at $T_{CO} \sim 100$ K is a charge-ordered (CO) state. The low temperature transition is often to a spin-Peierls (SP) state that appears at $T_{SP} \sim 10$ K, and that competes with the CO state. We have investigated the thermodynamics of these systems within an extended Hubbard Hamiltonian that includes (a) on-site and nearest neighbor Coulomb interactions, and (b) bond- and site-coupled quantum phonons. From calculations of charge, bond and spin-susceptibilities we are able to explain the transition from the CO to the SP phase. The CO state corresponds to the charge occupancy scheme $...1010...$ (where ’1’ and ’0’ denote charge-rich and charge-poor sites respectively), while the SP state has charge occupancy $...1100...$. The transition from the CO to the SP phase as temperature is lowered is driven by spin effects: At high temperatures, high-spin states dominate the free energy, and favor the $...1010...$ CO configuration. At low temperatures, spin singlet states dominate the free energy and instead favor a singlet SP state with the $...1100...$ charge pattern. In the temperature region $T_{SP} < T < T_{CO}$ there occur mixed spin-charge solitons that are domain walls between the $...1010...$ and $...1100...$ charge patterns.
11:27AM J11.00002 Finite-Temperature Phase Transitions in Quasi-One-Dimensional Molecular Conductors. HITOSHI SEO, Synchrotron Radiation Research Center, JAEA/SPRING-8, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo, TAKEDO KATO, Institute for Solid State Physics (ISSP), University of Tokyo — Phase transitions to symmetry-broken states in quarter-filled quasi-one-dimensional molecular conductors, such as DCNQI$_2$X, TMTTF$_2$X, and EDO-TTF$_2$X, are studied theoretically. We consider extended Hubbard chains with on-site, intra-chain, and inter-chain Coulomb interactions, coupled to the lattice degree of freedom by Peierls-type and Holstein-type electron-lattice interactions. We apply the numerical quantum transfer-matrix method to an effective one-dimensional model, treating the inter-chain term within mean-field approximation. Finite-temperature properties are investigated for the charge ordering, the dimer-type Mott transition (bond dimerization), and the spin-Peierls transition (bond tetramerization), by computing the temperature dependences of the order parameters together with those of the charge and spin susceptibilities. A coexistent state of charge order and bond dimerization exhibiting dielectricity is predicted in a certain parameter range, even when intrinsic dimerization is absent. Reference: H. Seo, Y. Motome and T. Kato, preprint(cond-mat/0611499) to be published in J. Phys. Soc. Jpn. 76 (2007) No. 1.

11:39AM J11.00003 Soliton Wall Superlattice Phase in Organic Conductor (Per)$_2$Pt(mnt)$_2$ in a Magnetic Field. SI WU, ANDREI LEBED, Dept. of Physics, University of Arizona — We suggest a model [1] to explain the appearance of a high resistance high magnetic field charge-density-wave (CDW) phase, discovered in quasi-one-dimensional (Q1D) organic conductor (Per)$_2$Pt(mnt)$_2$. In particular, we show that the Pauli spin-splitting effects improve the nesting properties of a realistic Q1D electron spectrum, and, therefore, a high resistance Peierls CDW phase is stabilized in high magnetic fields. In intermediate and very high magnetic fields, a periodic soliton wall superlattice (SWS) phase is found to be a ground state. We suggest to study the predicted phase transitions between the Peierls and SWS CDW phases to discover a unique SWS state. [1] A.G. Lebed and Si Wu, Physical Review Letters, submitted (2006).

11:51AM J11.00004 Nature of superconducting state in the new phase of (TMTSF)$_2$PF$_6$ under pressure. LEV GOR’KOV, NHMFL, Florida State University, PAVEL GRIGORIEV, Landau Institute for Theoretical Physics, RAS, Russia — The unusual phase has been recently observed in the organic material (TMTSF)$_2$PF$_6$, where superconductivity coexists with spin-density wave in the pressure interval $p_{c1}<p<p_{c2}$ below the first order transition into superconducting or normal metal phase. Assuming that the coexistence takes place on the microscopic scale, we consider the properties of the intermediate phase. We show that the new superconducting state inside spin-density wave phase just above $p_{c1}$ must bear a triplet pairing.

12:03PM J11.00005 Angular magnetoresistance oscillations in quasi-one-dimensional organic conductors in the presence of a crystal superstructure. ANAND BANERJEE, VICTOR YAKOVENKO, University of Maryland — Crystal superstructures, produced by anion ordering in the quasi-one-dimensional organic conductors (TMTSF)$_2$ReO$_4$ and (TMTSF)$_2$ClO$_4$, modify electron spectra in these materials and generate effective tunneling amplitudes between distant chains. These amplitudes cause multiple peaks in the interlayer conductivity for the magnetic field orientations along the rational crystallographic directions (the Lebed magic angles). The different wave vectors of anion ordering in (TMTSF)$_2$ReO$_4$ and (TMTSF)$_2$ClO$_4$ result in the odd and even Lebed angles, as observed experimentally. Reference: cond-mat/0608317.

12:15PM J11.00006 Angular and Temperature Dependent $^{77}$Se NMR in the Metallic and Field-Induced Spin Density Wave State in (TMTSF)$_2$ClO$_4$. LLOYD LUMATA, PHIL KUHNS, ARNEIL REYES, JAMES BROOKS, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310 — We present an exploratory investigation of the NMR pulse-power and magnetic field direction dependence of the $^{77}$Se NMR line shapes and relaxation rates in the metallic and field-induced spin density wave (FISDW) state of the quasi-one-dimensional organic conductor (TMTSF)$_2$ClO$_4$. By reducing the integrated NMR pulse power (via width and/or pulse height), the limitations of the enhancement factor below the FISDW transition are overcome, and the $^{77}$Se spin-lattice relaxation rate $1/T_1$ can be measured in both the metallic and FISDW states vs. temperature and field direction. Our results on the temperature dependence of $1/T_1$ in the vicinity of the FISDW transition, and also a description of the temperature and field direction dependence of the NMR spectra, will be presented.

1Work supported in part by NSF-DMR-0602859.

12:27PM J11.00007 Superconductivity in (TMTSF)$_2$ClO$_4$ probed by $^{77}$Se NMR. J. SHINAGAWA, UCLA, Y. KUROSAKI, University of Tokyo, S. E. BROWN, UCLA, D. JEROME, Universite de Paris, Sud, J. B. CHRISTENSEN, K. BECHGAARD, Orsted Institute, Copenhagen — Superconductivity in the Bechgaard salts (TMTSF)$_2$X, with X=PF$_6$, ClO$_4$, survives well beyond the paramagnetic limit set by the transition temperature $T_c \approx 1K$. As a result, it has been hypothesized that the spin pairing is triplet. We report on measurements of the $^{77}$Se Knight shift and spin-lattice relaxation rate $T_1^{-1}$, conducted in situ with interlayer resistivity, deep within the superconducting state of (TMTSF)$_2$ClO$_4$. At fields $H_0 \approx 10kOe$ aligned along the $a$- and $b'$-axes, the Knight shift reveals a decrease in spin susceptibility $\chi_s$ that is likely consistent with singlet pairing. The field dependence of $T_1^{-1}$ at temperatures $T \ll T_c$ exhibits a very sharply-defined increase at a field $H_s \approx 15kOe$. For $H_0 > H_s$, $T_1^{-1}$ is close to the normal state value, even though $H_d > H_s$. $R_{xx}$ is 0 to within experimental uncertainty. We discuss the implications for interpreting the results as evidence for a crossover, or a phase transition within the superconducting state.

12:39PM J11.00008 Angular Dependent Magnetoresistance Measurements of (Per)$_2$Au(mnt)$_2$ Under Pressure. D. GRAF, E.S. CHOI, J.S. BROOKS, NHMFL/FSU, Tallahassee, FL, M. ALMEIDA, Instituto Tecnologic o e Nuclear/CFMCUL, Sacavm, Portugal — The one-dimensional organic conductor (Per)$_2$Au(mnt)$_2$ has a charge density wave (CDW) ground state when cooled below a transition temperature of $T_{CDW} \sim 12 K$ under ambient pressure. The CDW state is largely suppressed by applying a pressure of $\sim 6 kbar$, as shown by a dramatic increase in low temperature conductivity where the behavior remains slightly activated, providing evidence of a mixed CDW-metal state. Oscillations under pressure are observed in the magnetoresistance (MR) which agree well with band structure estimates of the Fermi surface and are explained by Stark quantum interference. The angular dependence of the MR oscillations has been studied using the continuous rotation of a pressure cell in constant magnetic fields, aligned with the crystallographic planes of the sample. The results will be discussed within the context of known MR angular effects (i.e. Lebed or Danner-Kang-Chaikin oscillations) as well as the inhomogenous CDW-metal state which may exist in this pressure range.

2We acknowledge NSF-DMR 0602859 for support of this work and one of us (DG) also recognizes the NSF for fellowship support.
12:51PM J11.00009 Phase diagram of pressure-induced superconductor \(\beta-(\text{BDA-TPP})_2\text{MX}_4\) \((M=\text{Fe}, \text{Ga} \text{and } X=\text{Cl}, \text{Br})\) with localized magnetic moments\(^1\), E.S. CHOI, D. GRAF, T. TOKUMOTO, J.S. BROOKS, NHMFL/Florida State Univ., JUN-ICHI YAMADA, University of Hyogo — We have investigated transport and magnetization properties of \(\beta-(\text{BDA-TPP})_2\text{MX}_4\) \((M=\text{Fe}, \text{Ga} \text{and } X=\text{Cl}, \text{Br})\) as a function of pressure, temperature and magnetic field. The title material undergoes metal-insulator transitions above 100 K at ambient pressure. The insulating phase is suppressed with pressure and superconductivity eventually appears above \(P_c=4.5\) kbar \((X=\text{Cl})\) and 13 kbar \((X=\text{Br})\). The general temperature-pressure \((TP)\) phase diagram is similar each other, while higher pressure is required for \(X=\text{Br}\) compounds to suppress the insulating state and induce the superconductivity. Pressure dependent DC magnetization studies on \(\beta-(\text{BDA-TPP})_2\text{FeCl}_4\) compound revealed that the AFM ordering persist well above \(P_c\). In spite of similarity of phase diagram between \(M=\text{Fe}\) and \(M=\text{Ga}\) compounds, magnetoresistance results show distinct behaviors, which indicates the magnetic interaction with the conduction electrons are still effective. The comparison between \(X=\text{Cl}\) and \(X=\text{Br}\) compounds suggests the anion-size effect rather than the existence of localized magnetic moments plays more important role in determining the ground state.

\(^{1}\)We acknowledge NSF-DMR 0602859 for partial support for this work.

1:03PM J11.00010 High field ESR study of the \(pi-d\) interaction effect in beta-(BDA-TPP)_2MCl_4 \((M=\text{Fe, Ga})\), TAKAHISA TOKUMOTO, J. VANTOL, L. C. BRUNEL, E.S. CHOI, J.S. BROOKS, FSU/NHMFL, T. KAIHATSU, H. AKUTSU, J. YAMADA, U. of Hyogo — Novel magnetic organic conductors with \(pi-d\) interaction have commanded attention since the discovery of field induced superconductivity. One of them, beta-(BDA-TPP)_2FeCl_4, has alternating donor molecules and quasi 2D electrical properties. Previous studies of electrical and magnetic properties show an M-I transition at 120K and an AF transition at \(T_N=8.5K\), suggesting an exchange interaction between the conduction electrons and the Fe\(^{3+}\)-d electrons. The properties of beta-(BDA-TPP)_2GaCl_4 are similar with exception of the absence of the AF transition, which is apparently due to the absence of \(pi-d\) exchange interaction. We report angular/temperature dependent 240GHz quasi optical ESR measurements on both compounds to probe the magnetic properties. The Ga compound signals follow the donor molecule structure, and show no magnetic order at any temperature. The Fe compound signals are quite different from the Fe compound, and exhibit AF behavior below \(T_N\). The difference of Fe and Ga compounds will be discussed in terms of the interaction between localized and itinerant magnetic moments.

\(^{1}\)We acknowledge NSF-DMR 0602859 and 0520481 for support for this work.

1:15PM J11.00011 Metastable domains at the pressure induced neutral-ion transition of TTF-CA, ZOLTAN SOOS, Princeton University, ANNA PAINELLI, Parma University — Tetrathiafulvalene-Chloranil (TTF-CA) is the prototypical organic charge transfer (CT) salt whose neutral-ionic and dimerization (Peierls) transitions have been studied on cooling or under pressure. Volume changes switch the ground state from a band insulator with a fractional CT from TTF to CA of \(\rho=0.3\) in a regular stack to a Mott insulator with \(\rho>0.5\) in a dimerized stack. TTF-CA spectra indicate electron-vibration coupling to both lattice (e-ph) and molecular (e-mv) modes that lead to competing instabilities. Near the metallic point of the rigid system, a one-dimensional adiabatic Hubbard model with linear e-ph and e-mv coupling leads to metastable domains with different \(\rho, \rho'\) that are thermally accessible at 300 K over a limited bistability range. The transition of TTF-CA single crystals at 1 GPa indicates a pressure range with two resolved \(\rho, \rho'\). The model also describes the first order transition at 81 K at ambient pressure and generates anharmonic potential energy surfaces. These quantum transitions are driven by volume changes without contributions from electronic excited states.

1:27PM J11.00012 Mapping the temperature-dependent quasiparticle scattering rate over the Fermi surface of an organic superconductor\(^1\), JOHN SINGLETON, National High Magnetic Field Laboratory, Los Alamos, PAUL GODDARD, ARZHAM ARDÁN, STEPHEN BLUNDELL, Oxford University Physics, ROSS MCDONALD, National High Magnetic Field Laboratory, STAN TOZER, National High Magnetic Field Laboratory, Tallahassee, AMALIA COLDEA, Bristol University Physics, JOHN SCHLUETER, Argonne National Laboratory — The interlayer magnetoresistance \(\rho_{xz}\) of the organic metal \(\kappa-(\text{BEDT-TTF})_2\text{Cu(NCS)}_2\) is studied in fields of up to 45 T at and temperatures \(T\) from 0.5 K to 30 K. The peak in \(\rho_{xz}\) seen in planar fields, a definitive signature of interlayer coherence, remains to \(T\)'s exceeding the Anderson criterion for incoherent transport by a factor \(\sim 30\). Angle-dependent magnetoresistance oscillations are modeled using an approach based on field-induced quasiparticle paths on a 3D Fermi surface, to yield the \(T\) dependence of the scattering rate \(\tau^{-1}\). The results suggest that \(\tau^{-1}\) does not vary strongly over the Fermi surface, and that it has a \(T^2\) dependence due to electron-electron scattering. These findings are contrasted with recent experiments on cuprates, and their implications for models of organic superconductivity (e.g., FLEX) are discussed.

\(^{1}\)Supported by DOE, NSF, State of Florida and EPSRC (UK)

1:39PM J11.00013 ABSTRACT WITHDRAWN

1:51PM J11.00014 Coexisting fluctuations of charge ordering in quasi-2D organic conductors, \(\theta-(\text{ET})_2X\), MASAFUMI UDAGAWA, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo — Charge ordering is a crystallization of electrons driven by strong correlations, and is one of the central issues in organic conductors. In particular, the charge ordering in 1/4-filled quasi-2D materials, \(\theta-(\text{ET})_2X\), attracts much attention since the anisotropic triangular lattice structure enables us to study the stability of charge order under the geometrical frustration and quantum fluctuation. A systematic phase diagram was obtained for the anion \(X\) which controls the frustration, and surprisingly, an unusual coexistence of charge fluctuations with different wave numbers was observed in the quantum critical regime where the transition temperature goes to zero. Some exotic phenomena such as the strongly non-linear I-V characteristics and large magneto-resistance are observed in this regime, possibly induced by the anomalous properties of the charge degree of freedom. Here we theoretically study how the charge order and its fluctuations develop in the frustrated systems by applying the random-phase approximation to the extended Hubbard model with electron-phonon couplings. We successfully reproduce the coexisting charge fluctuations as well as the phase diagram. The coexistence originates from the competition between the kinetic energy and the Coulomb repulsion in the intermediate coherence regime, and is characteristic of the charge degree of freedom.

2:03PM J11.00015 Anisotropy of the competing superconducting and magnetic states in quasi-2D organic conductor \(\kappa-(\text{BEDT-TTF})_2\text{Cu[N(CN)]}_2\text{Br}\): An elastic investigation, D. FOURNIER, M. POIRIER, K.D. TRUONG, Département de Physique, Université de Sherbrooke, Qc, Canada — Ultrasound measurements performed on the quasi-2D organic conductor \(\kappa-(\text{BEDT-TTF})_2\text{Cu[N(CN)]}_2\text{Br}\) reveal a phase separation between superconductivity and magnetism in the vicinity of the Mott transition line. We report here longitudinal (L) and transverse (T) ultrasound measurements propagating perpendicular to the highly conducting planes; a magnetic field up to 18 Tesla could be applied along the same direction to differentiate the superconducting phase from the magnetic one. The huge velocity dip observed between 30 and 40 K and associated to a compressibility increase driven by the electronic degrees of freedom is not observed for T-waves polarized along \(001\); this implies that only magnetic fluctuations associated to 1D sheets of the Fermi surface can couple to the ultrasonic waves. Around \(T_c=12\) K, both the temperature profile and the amplitude of the elastic anomalies are highly dependent on the wave polarization. A magnetic field investigation of these anomalies not only establishes the anisotropic character of the superconducting anomaly, but it reveals also the onset of a magnetic transition below 15 K over the same temperature range as the superconducting one. These anomalies likely favor a multi-component superconducting order parameter.
Using Hanle techniques, we perform single electron Kerr rotation measurements at University of California, Santa Barbara, CA 93106 — Kerr rotation measurements are used to directly and non-destructively probe the dynamics of a single M.H. MIKKELSEN, J. BEREZOVSKY, O. GYWAT, N.G. STOLTZ, L.A. COLDREN, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Kerr rotation studies of single electron spin dynamics in a quantum dot.

In contrast, at larger charging rates, we find that which the charging rate of the dot is relatively low, the results yield a 1. InAs/GaAs[2], CdTe[3], and Ge/Si QDs[4] have also indicated size dependency. Using 8-band k.p theory, we calculated electric field dependent hole g-factors modulation of the g-factor by an electric field may permit spin manipulation for quantum information processing. Hole g-factors in quantum wells have a large anisotropy between the in-plane (g= 0) and growth (g=2.3) directions[1]. Calculations of hole g-factors for InAs/GaAs[2], CdTe[3], and Ge/Si QDs[4] have also indicated size dependency. Using 8-band k.p theory, we calculated electric field dependent hole g-factors on a variety of InAs/GaAs QDs. We find a large anisotropy: g=0.75 and 2.5 for B along (1-10) and (001) respectively for an elliptical dot with Eg=1.136, and g=0.059 and 2.8 for a round dot with Eg=1.133. A 100kV/cm field along (001) changes the (1-10) g-factor from 0.75 to 1.1 in the elliptical dot (0.059 to 0.058 for the round dot), and the (001) g-factor changes from 2.5 to 2.3 (2.8 to 2.9). [1] Sapega et al., PRB 45, 4320 (1992). [2] C. Pryor and M. E. Flatté, PRL 96, 026804 (2006). [3] Prado et al., PRB 69, 201310(R) (2004). [4] Nenashev et al., PRB 67, 205301 (2003).

11:51 AM J12.00002 Valley Kondo Effect in Silicon Quantum Dots, SHIU YEUAN SHIAU, SUCISMITA CHUTIA, ROBERT JOYNT, Physics Department, UW-Madison — Recent progress in the fabrication of quantum dots using silicon opens the prospect of observing the Kondo effect associated with the valley degree of freedom. We compute the dot density of states using an Anderson model with infinite Coulomb interaction U. The density of states is obtained as a function of temperature and applied magnetic field in the Kondo regime using an equation-of-motion approach to obtain the Green’s functions of the electrons. We predict the appearance of a very complex peak structure near the Fermi energy, much richer than the one or two peaks of the usual spin Kondo effect. We also show that the valley index is typically not conserved when electrons tunnel into a silicon dot. Analysis of the conductance should enable experimenters to understand the interplay of Zeeman splitting and valley splitting, as well as the dependence of tunneling on the valley degree of freedom.

12:03 PM J12.00003 Tuning Hole g-Factors in Self-Assembled InAs/GaAs Quantum Dots with an Electric Field, JOSEPH PINGENOT, CRAIG E. PRYOR, MICHAEL E. FLATTE, Optical Science and Technology Center, The University of Iowa — The g-factors of holes in quantum dots (QDs) determine the energy splittings of the spin states in a magnetic field, influencing spin precession, spin lifetimes, and photoluminescence polarization. Modulation of the g-factor by an electric field may permit spin manipulation for quantum information processing. Hole g-factors in quantum wells have a large anisotropy between the in-plane (g= 0) and growth (g=2.3) directions[1]. Calculations of hole g-factors for InAs/GaAs[2], CdTe[3], and Ge/Si QDs[4] have also indicated size dependency. Using 8-band k.p theory, we calculated electric field dependent hole g-factors on a variety of InAs/GaAs QDs. We find a large anisotropy: g=0.75 and 2.5 for B along (1-10) and (001) respectively for an elliptical dot with Eg=1.136, and g=0.059 and 2.8 for a round dot with Eg=1.133. A 100kV/cm field along (001) changes the (1-10) g-factor from 0.75 to 1.1 in the elliptical dot (0.059 to 0.058 for the round dot), and the (001) g-factor changes from 2.5 to 2.3 (2.8 to 2.9). [1] Sapega et al., PRB 45, 4320 (1992). [2] C. Pryor and M. E. Flatté, PRL 96, 026804 (2006). [3] Prado et al., PRB 69, 201310(R) (2004). [4] Nenashev et al., PRB 67, 205301 (2003).

12:15 PM J12.00004 Non-destructive Kerr rotation measurements of a single spin in a quantum dot, J. BEREZOVSKY, M.H. MIKKELSEN, O. GYWAT, N. STOLTZ, L. COLDREN, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — A single electron spin in a quantum dot forms a natural two state system for use in quantum information processing. The ability to measure this spin without destroying the system is an important step towards observing various quantum measurement-related phenomena. In contrast to previous experiments, we have performed non-destructive Kerr rotation measurements on a single electron spin confined in a charge-tunable semiconductor quantum dot. This measurement technique provides a means to directly probe the spin off-resonance, thus minimally disturbing the system. Energy-resolved Kerr rotation spectra demonstrate that we are probing a single electron, and also reveal information about the optically-pumped spin polarization as a function of quantum dot charging. These results point the way towards quantum non-demolition measurements and optically-mediated entanglement of spins in the solid state.

1 Work supported by NSF and AFOSR.

2 J. Berezovsky et al., Science Express, 9 November 2006, (10.1126/science.1133862).

12:27 PM J12.00005 Kerr rotation studies of single electron spin dynamics in a quantum dot, M.H. MIKKELSEN, J. BEREZOVSKY, O. GYWAT, N.G. STOLTZ, L.A. COLDREN, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Kerr rotation measurements are used to directly and non-destructively probe the dynamics of a single electron spin in a charge-tunable quantum dot[2]. The dot is formed by interface fluctuations of a GaAs quantum well and embedded in a vertical optical cavity. Using Hanle techniques, we perform single electron Kerr rotation measurements at $T = 10K$ in order to monitor the depolarization of an optically pumped electron spin within an applied transverse magnetic field. This reveals information about the time averaged transverse spin lifetime, $T_2^*$. At gate voltages for which the charging rate of the dot is relatively low, the results yield a $T_2^*$ in agreement with values expected from the hyperfine interaction in these materials. In contrast, at larger charging rates, we find that $T_2^*$ is strongly reduced, indicating the importance of additional decoherence mechanisms in that regime.

1 We acknowledge support from NSF and AFOSR.

12:39PM J12.00006 Driven coherent oscillations of a single electron spin in a quantum dot. FRANK KOPPENS, CHRISTO BUIZERT, KLAAS-JAN TIELROOIJ, IVO VINK, KATJA NOWACK, TRISTAN MEUNIER, LEON KOUWENHOVEN, LIEVEN VANDERSYPEN, Kavli Institute of Nanoscience Delft — The ability to control the quantum state of a single electron spin in a quantum dot is at the heart of recent developments towards a scalable spin-based quantum computer. In combination with the recently demonstrated controlled exchange gate between two neighbouring spins [1], driven coherent single spin rotations would permit universal quantum operations. In this talk, I will discuss the experimental realization of single electron spin rotations in a gate-defined GaAs double quantum dot. We coherently control the quantum state of the electron spin by applying short bursts of an on-chip generated oscillating magnetic field [2]. This allows us to observe up to eight Rabi oscillations of the electron spin in a microsecond burst. Via Ramsey-type pulse sequences we measure an apparent time-averaged coherence time which is limited by the hyperfine interaction with the nuclear spins. We erase these nuclear spin effects to a large extend via spin-echo pulse sequences and recover the intrinsic coherence time. [1] J.R. Petta et al., Science 309, 2180–2184 (2005). [2] F.H.L. Koppens et al., Nature 442, 766–771 (2006).

12:51PM J12.00007 Spin Coherence Modulated Triion Transitions and Probabilistic Initialization in Charged Semiconductor Quantum Dots1. YANWEN WU, ERIK KIM, XIAODONG XU, JUN CHENG, DUNCAN STEEL, The H. M. Randall Laboratory of Physics, University of Michigan, Ann Arbor, MI 48109, SOPHIA ECONOMOU, LU SHAM, Department of Physics, University of California, San Diego, La Jolla, California, 92039-0319, DAN GAMMON, ALAN BRACKER, The Naval Research Laboratory, Washington D.C. 20375 — The presence of symmetry breaking in a three-level \( \Lambda \) system consisting of two spin ground states and a charged exciton (trion) state leads to new features, where the population excited to the trion state is modulated by the spin coherence. This phenomenon is due to the unique semiconductor environment of the quantum dot (QD) system, which allows for two simultaneously orthogonal spinor axes. In addition, the polarization dependent excitations due to the double spinor axes of the system can be utilized to create a net spin from a completely mixed spin state, which is impossible to achieve through unitary operation of the spin system. This result provides an important application to the practical implementation of ultrafast spin based quantum computation in the semiconductor QD system in terms of qubit initialization.

1This work was supported in part by LPS, ARO, ONR, AFOSR and NSF-FOCUS.

1:03PM J12.00008 Radio frequency charge sensing and nuclear polarization of a two-electron double quantum dot1. DAVID REILLY, EDWARD LAIRD, Harvard University, JACOB TAYLOR, MIT, JASON PETTA, Harvard University / Princeton University, CHARLES MARCUS, Harvard University, MICAH HANSON, ART GOSSARD, University of California, Santa Barbara — We report charge-sensing measurements of a two-electron double quantum dot using an electrometer based on a radio-frequency quantum point contact (rf-QPC). In analogy with the radio frequency single electron transistor (rf-SET) the rf-QPC makes use of a LC impedance transformer and radio frequency reflectometry to achieve high charge sensitivity over a bandwidth exceeding 20MHz. In addition, we use controlled nanosecond pulsing of the double-dot potential to drive singlet to triplet transitions that develop a partial polarization of the nuclear spins. Using the rf-QPC, the subsequent diffusion and dynamics of nuclear polarization is examined on fast timescales.

1Support from DARPA-QUIST and ARO-STIC gratefully acknowledged.

1:15PM J12.00009 Fast spin state preparation in a single charged quantum dot3. XIAODONG XU, YANWEN WU, BO SUN, JUN CHENG, QIONG HUANG, DUNCAN STEEL, H. M. Randall Laboratory, The University of Michigan, Ann Arbor, MI 48109, USA, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington DC 20375, CLIVE EMARY, LU SHAM, Department of Physics, The University of California, San-Diego, La Jolla, California 92093 — Electron spins trapped inside of semiconductor dots (QD) are promising candidates for quantum bits (qubits). Quantum computation requires both the initialization of qubits with a high fidelity and a continuous supply of fresh ancillary qubits. The latter is the key for quantum error correction (QEC). Here, we demonstrate fast spin state preparation (laser cooling of an electron spin) in a single charged InAs self-assembled QD by applying magnetic field in the Voigt geometry. The preparation efficiency of the spin state is 98.9% at a magnetic field of 0.86T, which corresponds to the cooling of spin from 9 K (experimental temperature) to 0.06 K. To reach the same efficiency by thermal equilibration, a 69 T static magnetic field should be applied. The spin cooling rate of \( 3 \times 10^8 \text{s}^{-1} \) is achieved. This is three orders of magnitude faster than the spin decoherence rate, which is on the order of \( 10^{-3} \).

3This work is supported by U.S. ARO, AFOSR, ONR, LPS, and FOCUS-NSF.

1:27PM J12.00010 Exchange-controlled single-spin rotations in quantum dots. WILLIAM COISH, DANIEL LOSS, University of Basel — We show theoretically that arbitrary coherent rotations can be performed quickly (with a gating time \( \sim 1 \text{ ns} \)) and with high fidelity on the spin of a single electron confined to a quantum dot using exchange. These rotations can be performed using experimentally proven techniques for rapid exchange control, without the need for spin-orbit interaction or ac electromagnetic fields. We expect that implementations of this scheme would achieve gate error rates on the order of \( \eta \sim 10^{-3} \), within reach of several known error-correction schemes.

1:39PM J12.00011 Mixing of trion spin states in single and coupled dots from electron-hole and electron-electron exchange . S. C. BADescu, T. L. REINecke, U.S. Naval Research Laboratory, Washington DC — Polarized light spectroscopy is of interest for initializing and reading the electron (e) spin state in quantum dot (QD) systems for quantum information applications. An additional electron-hole (e-h) pair is created in the QD giving rise to a transient trion state [1]. The mechanisms behind the spin-conserving (asymmetric) e-e exchange and of the e-h exchange are important for understanding the spin dynamics of the trion. Here, first we show the importance of the long-range e-e exchange for the flip-flop mechanism in the lowest triplet of a single QD, particularly for highly-symmetric QDs. This adds to the strong e-e asymmetric exchange in a cylindrical QD [2]. Second, we consider a double-dot system, and we describe the combined effect of e-h and e-e asymmetric exchange in the lowest (delocalized) triplet by comparison to the first excited (localized) triplet [1] M. E. Ware et al., PRL 95(17), 177403 (2005) [2] S. C. Badescu and T. L. Reinecke, cond-mat/0610405

5:15PM J12.00012 Electric Dipole Spin Resonance for Heavy Holes in Quantum Dots1. DENIS BULAEV, DANIEL LOSS, Institute of Physics, University of Basel, CH-4056 Basel, Switzerland — We propose and analyze a new method for manipulation of a heavy hole spin in a quantum dot. Due to spin-orbit coupling between states with different orbital momenta and opposite spin orientations, an applied rf electric field induces transitions between spin-up and spin-down states. This scheme can be used for detection of heavy-hole spin resonance signals, for the control of the spin dynamics in two-dimensional systems, and for determining important parameters of heavy-holes such as the effective \( g \)-factor, mass, spin-orbit coupling constants, spin relaxation and decoherence times.

1We acknowledge support from the Swiss NSF, NCCR Nanoscience, DARPA, ONR, and JST ICORP.

Tuesday, March 6, 2007 11:15AM - 2:15PM –
Session J13 DMP GMAG: Focus Session: Multiferroics III Colorado Convention Center Korbel 4C

11:15AM J13.00001 Interatomic spin-orbit coupling: mechanism for spin-spiral-caused ferroelectricity. T.A. KAPLAN, S.D. MAHANTI, Michigan State University — There are two general classes of mechanisms that have been proposed for spin-spiral caused ferroelectricity, one based on ionic displacements as primary cause, the other on charge distortion without ionic displacements. Here we discuss the latter1,2. The model proposed here is illustrated by a model where a pair of ions a and b each have low-lying s- and excited p- states with a prescribed spin state s_a for the a-site states, similarly for the b-site, and there are 2 electrons; interatomic spin orbit coupling resides in inter-ion hopping due to s-p matrix elements of the spin-orbit coupling operator \( \propto S\cdot \sigma \cdot \gamma \cdot \sigma \cdot \gamma \cdot \sigma \) where \( S\) is a unit vector in the direction of spin at the site. For the a-site states, similarly for the b-site, and there are 2 electrons; interatomic spin orbit coupling resides in inter-ion hopping due to s-p matrix elements of the spin-orbit coupling operator \( \propto S\cdot \sigma \cdot \gamma \cdot \sigma \cdot \gamma \cdot \sigma \) where \( S\) is a unit vector in the direction of spin at the site. As was found when there is a coi1,2. For the spins in a chain parallel to the spiral wave vector in CoCrO_2, direction [110], results in ferroelectricity, as observed1; the spins in a [1,0,0]-directed chain, give an antiferroelectric component. Extension to a pair of Cr\(^{2+}\) ions will be discussed.

2. T. A. Kaplan and S. D. Mahanti, cond-mat/0608227, 10 Aug 2006

11:27AM J13.00002 Magnetoelectric properties of cobalt oxides with low dimensional structures. H. KUWAHARA, M. AKAKI, K. NODA, F. NAKAMURA, D. AKAHOSHI, Sophia Univ. — Since the discovery of novel ferroelectric transition due to spiral spin structures in TbMnO_3, the subject compound, BaCo_2Si_2O_6, resultantly exhibit nontrivial spin structures. In this work, we have investigated the magnetic and dielectric properties of cobalt oxides with low dimensional structures. The subject compound, BaCo_2Si_2O_6 single crystal, is a derivative from Ba_2Cu_2O_3 in which the spiral spin structure is reported below 3.26K. We have substituted Co\(^{2+}\) for Cu\(^{2+}\) to increase the transition temperature. The crystallographic symmetry of the obtained crystal at RT was confirmed to be C2/c which does not break the inversion symmetry. The Weiss temperatures estimated in paramagnetic region are \(-20K\) (H||c) and \(-74K\) (H||c), indicating the large magnetic anisotropy. The weak ferromagnetization rises up at 21K, where the dielectric constant perpendicular to the c axis \(\varepsilon_{\perp}\) decreases concomitantly. In addition, we have observed the magnetocapacitance effect below 21K: \(\Delta\varepsilon_{\perp}(20K, H||c) \geq 0.2\%\) at 5.5K. This result suggests that there exists a coupling between magnetism and dielectricity. Results of Ba_2CoSi_2O_6 will also be presented.

11:39AM J13.00003 Ferroelectricity in a quantum chain magnet. S. PARK, Y.J. CHOI, C.L. ZHANG, S-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics & Astronomy, Rutgers University, Piscataway, New Jersey 08854 — Multiferroics with enhanced cross-coupling effects exhibit magnetic orders with broken centrosymmetry. It turns out that the lattice relaxation through exchange striction associated with the magnetic orders with non-centrocymetry is the origin of magnetism-induced ferroelectricity. Among the exchange strictions, the Dzyaloshinskii-Moriya type interaction becomes active when ferroelectricity is induced by spiral magnetic orders. Herein, we report our surprising discovery that a quantum chain magnet exhibits ferroelectricity when the spiral magnetic order sets in.

11:51AM J13.00004 Direct transition from a disordered to a multiferroic phase. MICHEL KENZELMANN, ETH Zurich, GAIVIN LAWES, Wayne State University, BROOKS HARRISON, University of Pennsylvania, GASPAROVIC GORAN, National Institute of Standards and Technology, Gaithersburg, BROHOM COLLIN, Johns Hopkins University, ART RAMIREZ, Bell Labs, Lucent Technologies, G.A. JORGE, MARCEO JAIME, Los Alamos National Laboratory, SUNGIL PARK, HANARO Center, Korea, A. YA. SHAPIRO, L. A. DEMIANETS, A.V. Shubnikov Inst for Crystallography, Moscow. — We report the first direct transition from a paramagnetic and paraelectric phase to an incommensurate multiferroic in a triangular lattice antiferromagnet. Ferroelectricity is only observed when the magnetic structure has chirality and breaks inversion symmetry. A magnetic field extinguishes the electric polarization through a change in the magnetic symmetry. A Landau expansion of symmetry-allowed terms in the free energy demonstrates that the magnetic ordering of the triangular lattice antiferromagnet gives rise to a pseudoelectric field, whose temperature dependence agrees with that of the observed electric polarization. The observed multiferroic behavior provides a theoretically tractable example of ferroelectricity from competing spin interactions.

12:03PM J13.00005 Mapping Structural Phase Separation in Eu_0.5Y_0.5MnO_3 using 3D X-ray Microdiffraction. J.D. BUDAI, J.Z. TISCHLER, ORNL, W. LIU, ANL, D.D. SARMA, D. TOPWAL, Ind. Inst. Sci., G. SHENOY, W. YANG, ANL, B.C. LARSON, ORNL, S-W. CHEONG, Rutgers Univ., A.A. MUKHIN, Russ. Acad. Sci. — Phase coexistence in multicomponent manganite systems is known to occur over a wide range of length scales and strongly influences the magnetic and electronic properties. We have used 3D synchrotron x-ray microdiffraction to investigate domain formation and local lattice structure in bulk Eu_0.5Y_0.5MnO_3 single-crystals. X-ray microdiffraction yields 3D spatially-resolved maps of the crystal structure, orientation and lattice parameter, while microfluorescence yields depth-integrated composition maps. The x-ray microdiffraction patterns reveal alternating lamella of orthorhombic Eu-rich and hexagonal Y-rich phases with a self-organized periodicity of \(\sim\)15 microns. Both phases maintain a well-defined long-range (\(\sim\)mm) average crystal orientation with respect to the growth direction and to each other. However, small local variations in both orientation (i.e. mosaic) and lattice parameter (strain and composition) are observed, and the possible origins and implications of these inhomogeneities will be discussed.

1Support by DOE Office of Basic Energy Sciences, Division of Materials Sciences under contract with ORNL, managed by UT-Battelle; UNICAT/XOR and APS supported by DOE
Resonant magnetic scattering of multiferroic HoMnO$_3$. S. NANDI, A. KREYSSIG, L. TAN, J.-W. KIM, J.Q. YAN, R.J. MCQUEENEE, P.C. CANFIELD, A.I. GOLDMAN. Dept. of Physics, Iowa State University, IA 50011, A. BARCZA, Institute for Phy. Chem., University of Vienna, Austria — The multiferroic material HoMnO$_3$ displays electrical polarization below the Curie temperature $T_C = 875$ K and antiferromagnetic Mn$^{3+}$ ordering at Néel temperature, $T_N = 75$ K. The ferroelectric phase possesses hexagonal P6$_3$cm symmetry with polarization $P_z = 5.6 \mu$C cm$^{-2}$ along the hexagonal c axis. In order to shed further light on the magnetic order in this compound, element specific X-ray resonant magnetic scattering was performed at the Ho $L_{III}$ absorption edge. Resonance enhancement was observed in both quadrupole and dipole channels below 40 K. Measurement of $(001)$ and $(100)$ (1 odd) reflections have resolved contradictions present in the literature regarding the magnetic order of Ho$^{3+}$ moments. From 40 K down to 6 K, Ho$^{3+}$ moments order according to magnetic space group P6$_3$cm with different values for the ordered moment on the Wyckoff sites 2a and 4b. According to this space group, Ho moments are ferromagnetically correlated in the ab-planes and antiferromagnetically correlated in the c-direction.

The coincidence of the transition temperature (40 K) for Ho$^{3+}$ moment ordering, spin rotation for Mn$^{3+}$ moments, and sharp anomaly in dielectric constant indicates that the interplay between ferroelectricity and magnetism is strongly related to the Ho magnetic order.

Crystal Field Excitations in Multiferroic HoMnO$_3$. OWEN VAIJK, University of Missouri-Columbia, MICHEL KENZELMANN, JEFF LYNN, SUNG-BAEK KIM, SANG-WOOK CHEONG — Antiferromagnetic and ferroelectric order coexist in hexagonal HoMnO$_3$, and strong coupling between these two order parameters has been previously observed. Neutron scattering measurements of the low-energy excitations in HoMnO$_3$ reveal a complex spectra of Ho$^{3+}$ crystal-field excitations which depend upon both temperature and applied magnetic field. These crystal-field excitations are correlated with changes in the magnetic symmetry of the Mn$^{3+}$ magnetic sublattice. Measurements of the magnon excitation frequencies near these crystal field levels indicate strong coupling between the Mn$^{3+}$ moments and the Ho$^{3+}$ crystal field levels. This coupling may play a critical role in explaining the interaction of ferroelectricity and antiferromagnetism in HoMnO$_3$.

Resonance magnetic scattering of multiferroic HoMnO$_3$. J.-H. PARK, POSTECH, D.-Y. CHO, SNU, J.-Y. KIM, PAL, B.-G. PARK, K.-J. RHO, POSTECH, H.-J. NOH, B.-J. KIM, S.-J. OH, SNU, H.-M. PARK, KYUNG, J.-S. AHN, H. ISHIBASHI, S.-W. CHEONG, Rutgers University, J. H. LEE, P. MURUGAVELO, T. W. NOH, SNU, A. TANAKA, T. JO, Hiroshima University — Recently, multiferroicity, in which magnetism and ferroelectricity coexist, has attracted much attention due to its exotic magnetoelectric (ME) phenomena. Hexagonal $R=$ Ho, Er, with $T_{me}$ = 5.6 K, etc. These compounds show a complex mix of magnetic and ferroelectric symmetry below $T_N$. We observed that hexagonal TbMnO$_3$ exhibits excitations associated with the polarization dependent $\gamma$-ray absorption spectroscopy (PXAS) at O K- and Mn L$_2$,3-edges. PXAS exhibits strong polarization dependence at both edges, reflecting anisotropic Mn 3d orbital occupation. Moreover, the O K-edge spectra show that Y id states are strongly hybridized with O 2p ones, resulting in large anomalies in Born effective charges on off-centering Y- and O-ions. These results manifest that the Y $\delta$-ness with re-hybridization is the driving force for the ferroelectricity, and suggest a new approach to understand the multiferroicity in the hexagonal manganites.

Spin-lattice coupling in RMnO$_3$. J.-H. YEN, Ames Laboratory, R. J. MCQUEENEE, Department of Physics and Astronomy, Iowa State University, IA 50011, Y. REN, Argonne National Laboratory, J.-S. ZHOU, Texas Materials Institute, the University of Texas at Austin, J. B. GOODENOUGH, Texas Materials Institute, the University of Texas at Austin, Austin TX 78712 — The magnetic order in RMnO$_3$ (R=rare earth and Y) perovskites is quite sensitive to the R$^{3+}$ ionic radius. Type A magnetic order has been observed for R=Gd and La. For R=Dy and Tb, no classic magnetic order was observed down to the lowest temperature. The rest members of the family show a type E magnetic order. As far as we know, the lattice response to the magnetic order has not been systematically studied. Here we will discuss the lattice response to the magnetic order studied by synchrotron x-ray powder diffraction and thermal conductivity.

Epitaxially stabilized hexagonal TbMnO$_3$ thin films. DAESU LEE, JUNG-HYUK LEE, PATTUKKANNU MURUGAVEL, HYEJIN RYU, TAE WON NOH, ReCOE & FPRD, Department of Physics and Astronomy, Seoul National University, JAE WOOK KIM, HYUNG JIN KIM, KEE HOON KIM, CSCMR, Department of Physics and Astronomy, Seoul National University, YOUNGHUN JO, MYUNG-HWA JUNG, Quantum Material Research Team, Korea Basic Science Institute, JONG-GUL YOON, Department of Physics, University of Suwon, JIN-SEOK CHUNG, Department of Physics and CAMDRC, Soongsil University — We observed that hexagonal TbMnO$_3$ thin films showed multiferroic properties with enhanced ferroelectricity. The hexagonal TbMnO$_3$ thin film shows 1.6 $\mu$C cm$^{-2}$ as the remnant polarization value, which is 20 times larger than that of its orthorhombic bulk phase. In addition, the ferroelectric Curie temperature is shifted to 60 K compared to the low temperature value (27 K) of its bulk orthorhombic phase. Interestingly, the hexagonal TbMnO$_3$ film displayed the emergence of a new antiferroelectric-like phase just above 65 K, which is the first of its kind in the family of multiferroic hexagonal manganites. A clear anomaly in dielectric constant near the antiferromagnetic Neel temperature ($T_N$ <70 K) shows the possible coupling between the spin and charge degrees of freedom. This is indeed confirmed by the observed second-order magnetoelectric effect below $T_N$.

Spin structures of magnetic phases in magnetic ferroelectrics, RMnZ05 (R = Y and Tb). J.H. KIM, S.-H. LEE, Department of Physics, University of Virginia. J.-H. CHUNG, NIST Center for Neutron Research and Univ. of Maryland, M. KENZELMANN, ETH/PSI, J. SCHEFER, PSI, C.F. MAJKRZAK, NIST, S. PARK, S.-W. CHEONG, Rutgers University — We report polarized and unpolarized neutron diffraction data obtained from single crystals of magnetic ferroelectrics, RMnZ05 (R=Y and Tb). Each system undergoes, upon cooling, more than one magnetic and ferroelectric phase transition. By using the group representation theory and fitting the data, we have determined the spin structures of the different phases to elucidate the microscopic mechanism of the static spin-charge coupling in the multiferroics. Our results show that the magnet and ferroelectric phases of the two systems have spin structures that can only be constructed by a linear combination of the basis functions of two two-dimensional representations of the magnetic space group. Implication of the spin structures to the electric polarization of the systems and to theoretical models will also be discussed.

Magnetic excitations in magnetic ferroelectrics, RMnO$_2$. S. NANDI, A. KREYSSIG, L. TAN, J.-W. KIM, J.Q. YAN, R.J. MCQUEENEE, P.C. CANFIELD, A.I. GOLDMAN. Dept. of Physics, Iowa State University, IA 50011, A. BARCZA, Institute for Phy. Chem., University of Vienna, Austria — The multiferroic material HoMnO$_3$ displays electrical polarization below the Curie temperature $T_C = 875$ K and antiferromagnetic Mn$^{3+}$ ordering at Néel temperature, $T_N = 75$ K. The ferroelectric phase possesses hexagonal P6$_3$cm symmetry with polarization $P_z = 5.6 \mu$C cm$^{-2}$ along the hexagonal c axis. In order to shed further light on the magnetic order in this compound, element specific X-ray resonant magnetic scattering was performed at the Ho $L_{III}$ absorption edge. Resonance enhancement was observed in both quadrupole and dipole channels below 40 K. Measurement of $(001)$ and $(100)$ (1 odd) reflections have resolved contradictions present in the literature regarding the magnetic order of Ho$^{3+}$ moments. From 40 K down to 6 K, Ho$^{3+}$ moments order according to magnetic space group P6$_3$cm with different values for the ordered moment on the Wyckoff sites 2a and 4b. According to this space group, Ho moments are ferromagnetically correlated in the ab-planes and antiferromagnetically correlated in the c-direction.

The coincidence of the transition temperature (40 K) for Ho$^{3+}$ moment ordering, spin rotation for Mn$^{3+}$ moments, and sharp anomaly in dielectric constant indicates that the interplay between ferroelectricity and magnetism is strongly related to the Ho magnetic order.
11:39AM J14.00003 Thermally-Assisted Current-Driven Domain Wall Motion , REMBERT DUINE, Utrecht University, ALVARO NUNEZ, Valparaiso, Chile, ALLAN MACDONALD, The University of Texas of Austin — Starting from the stochastic Landau-Lifschitz-Gilbert equation, we derive Langevin equations that describe the nonzero-temperature dynamics of a rigid domain wall. We derive an expression for the average drift velocity of the domain wall $\langle v_{dw} \rangle$ as a function of the applied current, and find qualitative agreement with recent magnetic semiconductor experiments. Our model implies that at any nonzero temperature $T_{dw}$ initially varies linearly with current, even in the absence of non-adiabatic spin torques.
11:51AM J14.00004 Oscillatory dependence of current driven domain wall motion on current pulse length

LUc THOMAS, IBM Almaden Research Center — The motion of domain walls (DW) in magnetic nanowires driven by spin torque from spin-polarized current is of considerable interest. Most previous work has considered the effect of dc or ∼microsecond long current pulses. Here, we show that the dynamics of DWs driven by nanosecond-long current pulses is unexpectedly complex. In particular, we show that the current driven motion of a DW, confined to a pinning site in a permalloy nanowire, exhibits an oscillatory dependence on the current pulse length with a period of just a few nanoseconds [1]. This behavior can be understood within a surprisingly straightforward one dimensional analytical model of the DW’s motion. When a current pulse is applied, the DW’s position oscillates within the pinning potential out of phase with the DW’s out-of-plane magnetization, where the latter acts like the DW’s momentum. Thus, the current driven motion of the DW is akin to a harmonic oscillator, whose frequency is determined by the “mass” of the DW and where the restoring force is related to the slope of the pinning potential. Remarkably, when the current pulse is turned off during phases of the DW motion when it has enough momentum, the amplitude of the oscillations can be amplified such that the DW exits the pinning potential well after the pulse is turned off. This oscilatory depinning occurs for currents smaller than the dc threshold current, and, moreover, the DW moves against the electron flow, opposite to the propagation direction above the dc threshold. These effects can be further amplified by using trains of current pulses whose lengths and separations are matched to the DW’s oscillation period. In this way, we have demonstrated a five fold reduction in the threshold current required to move a DW out of a pinning site, making this effect potentially important for technological applications. [1] L. Thomas, M. Hayashi, X. Jiang, R. Moriya, C. Rettner and S.S.P. Parkin, Nature 443, 197 (2006).

1 In collaboration with Masamitsu Hayashi, Rai Moriya, Charles Rettner, Xin Jiang, Bastiaan Bergman, Brian Hughes and Stuart Parkin

12:27PM J14.00005 Spin-Transfer-Torque-Driven Domain-Wall Dynamics in Permalloy Nanowires

SHUQIANG YANG, JAMES ERSKINE, University of Texas at Austin — Pulse-current-driven domain-wall dynamics in Permalloy nanowires are studied using high-temporal-resolution magneto-optical techniques. The time-resolved measurements elucidate mechanisms responsible for stochastic variation in pulse-current-stimulated wall displacements, and resolve factor-of-10 disagreements between prior experimental [1,2] and theoretical determinations [3] of domain-wall velocity and spin-flip efficiency in magnetic nanowire structures. Current pulses with different width and amplitude are used to probe the domain-wall motion. By reducing the pulse width, higher excitation densities can be achieved, leading to more complex domain structures (probed by MFM) in the final state. [1] A. Yamaguchi et al. PRL 92, 077205-1, 2004 [2] M. Klau et al. PRL 95, 026601-1, 2005 [3] Z. Li and S. Zhang, PRL 92, 207203-1, 2004

Acknowledgment: Research supported by NSF DMR.0404252 (NIRT) and by R.A. Welch Foundation (F-1015).

12:39PM J14.00006 Coherent precession of propagating domain walls in permalloy nanowires

MASAMITSU HAYASHI, LUC THOMAS, CHARLES RETTNER, RAI MORIYA, STUART PARKIN, IBM Almaden Research Center — We report on domain wall (DW) dynamics in permalloy nanowires. We demonstrate the precessional nature of the DW propagation above the Walker breakdown field. Time resolved resistance measurements were performed on 200 nm wide 10 nm thick permalloy nanowires. Oscillations in resistance are observed when the DW propagates along the nanowire. The frequency of this oscillation varies linearly with magnetic field, according to the Larmor precession frequency. By contrast, current passing through the nanowire has relatively little effect on the oscillation frequency even though it is large enough to influence the DW velocity. To explore the origin of this resistance oscillation, dc resistance measurements were performed on permalloy nanowires with a pinning center located along the nanowire. The state of the DW pinned at the pinning center can be inferred from the nanowire’s resistance. By using a combination of current and magnetic field, the time at which the DW arrives at the pining center can be tuned, allowing us to show that the chirality of the domain walls reverses periodically as the wall propagates along the nanowire.

12:51PM J14.00007 Damping in Ferromagnets: Landau-Lifshitz versus Gilbert

WAYNE M. SASLOW, Texas A&M University, College Station TX 77843-4242, MARK D. STILES, NIST, Gaithersburg, MD 20899-8412, ANDREW ZANGWILL, School of Physics and Astronomy, Georgia Institute of Technology, Atlanta, GA 30332-0430 — We present the first fully quantum mechanical calculation of the spin flip interaction between spin polarized current and local spin systems. Dynamics of local spins will be illustrated as many electrons pass through the chain. The talk will focus on the description of the approach, density matrix formalism used in the calculations and the behavior of the system for different configurations. The interplay between electron-spin and spin-spin interaction, effect of domain walls, limiting cases for interaction strengths, spin degree of freedom, and comparison to LLG model will be presented.

Acknowledgment: Research supported by DOE grants DE-FG02-06ER46278 and DE-FG02-06ER46278.

11:03PM J14.00008 Interactions between spin-polarized current and local spin systems: A Quantum Mechanical Approach

FATIH DOGAN, Dept. of Physics, University of Alberta, Edmonton, AB, Canada, LUCIAN COVACI, Dept of Physics, University of British Columbia, Vancouver, BC, Canada, WONKEE KIM, FRANK MARSIGLIO, Dept. of Physics, University of Alberta, Edmonton, AB, Canada — In this talk, we present the first fully quantum mechanical calculation of the spin flip interaction between spin polarized current and local spin systems. Dynamics of local spins will be illustrated as many electrons pass through the chain. The talk will focus on the description of the approach, density matrix formalism used in the calculations and the behavior of the system for different configurations. The interplay between electron-spin and spin-spin interaction, effect of domain walls, limiting cases for interaction strengths, spin degree of freedom, and comparison to LLG model will be presented.

11:15PM J14.00009 Giant voltage response to magnetic field of model granular magnetic films and spin mixing effects

JEAN-PHILIPPE ANSERMET, M. HILLENKAMP, G. DIDOMENICANTONIO, C. FELIX, L. GRAVIER, S. SERRANO-GUISAN, M. ABID, EFPL — Magneto-thermogalvanic voltage (MTGV) is the magnetic field dependence of the AC voltage measured across a local spin system. We show that MTGV is a specific local spin system effect. We perform a full one dimensional quantum Monte Carlo simulation to study the MTGV in a granular magnetic film. The film consists of ferromagnetic nanoclusters embedded in a non-magnetic matrix. The nanoclusters have different sizes, and their orientation is random. We demonstrate that MTGV shows a giant response to magnetic field. MTGV is observed in all the nanoclusters. Furthermore, we find a strong correlation between the MTGV behavior and the spin flipping process in the nanoclusters. The MTGV signal is a superposition of MTGV signals from individual nanoclusters. In collaboration with Masamitsu Hayashi, Rai Moriya, Charles Rettner, Xin Jiang, Bastiaan Bergman, Brian Hughes and Stuart Parkin

1 In collaboration with Masamitsu Hayashi, Rai Moriya, Charles Rettner, Xin Jiang, Bastiaan Bergman, Brian Hughes and Stuart Parkin

1:27PM J14.00010 Dynamics of spin flipping

LUCIAN COVACI, University of British Columbia, WONKEE KIM, FATIH DOGAN, FRANK MARSIGLIO, University of Alberta — Interactions between a spin polarized current and a ferromagnetic spin chain will lead to the eventual flipping of the spins. We study the dynamics of spin flipping due to Kondo-like interactions between an electron and a spin chain. Interactions within the chain are taken to be of Heisenberg type. The full time dependent quantum mechanical problem is solved within a density matrix formulation. We present the time evolution of the electron wave packet and of the spin expectation values as the electron passes through the chain. The electron transmission probability is calculated as a function of electron momentum and interaction coupling strength. We observe excitations induced by spin transfer and resonant transmission regimes. Deviations from quasi-classical treatments of magnetic moments are discussed.
1:39PM J14.00011 Non-Equilibrium Spin Dynamics in the Subpicosecond Regime. ADNAN REBEI, Seagate Technology — Femto-second laser pulses are becoming an important tool that allows us to explore non-equilibrium spin dynamics at short time (high frequency) scales [1]. It has therefore become apparent [2] that more rigorous treatments are needed to correctly address spin relaxation at these energies. I will show how functional-methods of calculations of correlation energies in electron gas [3] can be successfully adapted to the problem of relaxation in magnetic systems [4]. The study of short time response entails a careful treatment of initial conditions. Our formalism naturally takes care of this and avoids the assumption that the system has been in equilibrium in the infinite past, an assumption common in Boltzmann-type treatments. As an example, we discuss possible non-equilibrium effects due to ultrasonic attenuation on spin relaxation when the magnon sub-system is initially near the Curie point.


1:51PM J14.00012 Thermal hysteresis in transport properties of chromium films due to Spin Density Wave (SDW) quantization and Domain-wall scattering. RAVI K. KUMMAMURU, YEONG-AH SOH, Dartmouth College, DEPARTMENT OF PHYSICS AND ASTRONOMY, DARTMOUTH COLLEGE, HANOVER, NH 03755 TEAM — Magnetotransport measurements were made on four Cr films of thicknesses 3500Å, 560Å, 430Å and 175Å sputtered on MgO substrates. We observe thermal hysteresis in the resistivity and Hall coefficient. Two types of hysteresis are observed, one in a temperature range of tens of Kelvin above 200 K and the other from the Neel temperature down to about 50 K. The first type is seen in the films, 175Å and 560Å. By looking at the Hall conductance in the vicinity of this hysteresis, we show that it arises directly from the SDW. The second type of hysteresis is absent in the thinnest 175Å film, but increases in magnitude with film thickness, and resistivity is always higher during cooling than warming. We conclude that the first type of hysteresis is caused due to discrete changes in the number of incommensurate SDW nodes due to confinement in the thickness dimension, and the second type is caused due to changes in the domain wall configuration with temperature, leading to a reduction in anti-ferromagnetic (AFM) SDW domain wall scattering.

Tuesday, March 6, 2007 11:15AM - 2:15PM
Session J16 GMAG DMP: Focus Session: Molecular Magnets
Colorado Convention Center Korbel 4F

11:15AM J16.00001 Interactions Between Thin Metallic Films and Mn12-Acetate.† Joel MEANS, WINFRIED TEIZER, Texas A and M University, Dept. of Physics, KIM R. DUNBAR, Texas A and M University, Dept. of Chemistry — Single-molecule magnets are a novel class of materials which have been extensively studied in recent years. One such molecule is Mn12-Acetate, [Mn12O12(CH3COO)12(H2O)4]4+·H2O, which exhibit photosinduced magnetism and, for the largest particles, long-range ferrimagnetic with finite coercive fields. The synthesis involves the variation of the concentration of the poly(vinylpyrrolidone), PVP, the encapsulating polymer, which controls the resulting particle size. From HR-TEM, the particle size distributions have been obtained for four batches of samples, with mean diameters ranging from nominally 3 nm to 13 nm. Upon irradiation with white light at 5 K, all samples exhibit photoinduced magnetism. Magnetization studies indicate that the smallest particles are superparamagnetic, while the largest ones are ferrimagnetic with long-range ordering temperatures (Tc ∼17 K) and coercive fields (HC ∼250 G) varying with particle size in a manner consistent with the predictions of finite-size scaling.

† The authors thank the Robert A. Welch Foundation (A-1585) and Sandia National Labs (Sandia Excellence in Science Fellowship) for financial support.

11:27AM J16.00002 Magnetism of Rubidium Cobalt Hexacyanoferrate Nanoparticles.†, D.M. PAJEROWSKI, M.W. MEISEL, Department of Physics, University of Florida, F.A. FRYE, D.R. TALHAM, Department of Chemistry, University of Florida — Although photoinduced magnetism in nanoparticles of Prussian blue analogs has been reported, these samples are superparamagnetic. We have generated and characterized nanoparticles of RbCo3[Fe(CN)6]3·nH2O, which exhibit photosinduced magnetism and, for the largest particles, long-range ferrimagnetic with finite coercive fields. The synthesis involves the variation of the concentration of the poly(vinylpyrrolidone), PVP, the encapsulating polymer, which controls the resulting particle size. From HR-TEM, the particle size distributions have been obtained for four batches of samples, with mean diameters ranging from nominally 3 nm to 13 nm. Upon irradiation with white light at 5 K, all samples exhibit photoinduced magnetism. Magnetization studies indicate that the smallest particles are superparamagnetic, while the largest ones are ferrimagnetic with long-range ordering temperatures (Tc ∼17 K) and coercive fields (HC ∼250 G) varying with particle size in a manner consistent with the predictions of finite-size scaling.

† Supported by NSF DMR-0305371 (MWM) and DMR-0543362 (DRT).

11:39AM J16.00003 Fabrication of nano-gapped single-electron transistors for transport studies of individual single-molecule magnets. CHRISTOPHER RAMSEY, JOHN HEMDERSON, ENRIQUE DEL BARCO, Dept. of Physics, University of Central Florida, ABHUDAYA MISHRA, GEORGE CHRISTOU, Dept. of Chemistry, University of Florida — Three terminal single-electron transistor devices utilizing Al/AO23 insulating layer. The single-electron transistor devices were then treated with O2 plasma and Mn12-(3-thiophenecarboxylate) SMMs were self-assembled on the surface. These molecules are Mn12-acetate derivatives, which have been functionalized with thiophene groups and are known to attach to Au surfaces. Self-assembly of the molecules was verified using scanning probe microscopy and XPS measurements. Nano-gapped electrodes were produced at low temperature by electromigration of the 90 nm wide Au wire, reliably yielding 1-3 nm gaps in which the SMM can be situated. We show that the nano-gap spacing can be fine tuned by adding resistance in series with the nanowire. Electron transport measurements were then performed to reveal gate dependent low level (less than 40 meV) excitations in the conductance of a single Mn12 SMM.
11:51 AM J16.00004 Will spin-relaxation times in molecular magnets permit quantum information processing? , ARZHANG ARDAVAN, Department of Physics, University of Oxford — Certain computational tasks can be efficiently implemented using quantum logic, in which the information-carrying elements are permitted to exist in quantum superpositions. To achieve this in practice, a physical system that is suitable for embodying quantum bits (qubits) must be identified. Some proposed scenarios employ electron spins in the solid state, for example phosphorous donors in silicon, quantum dots, heterostructures and endohedral fullerenes, motivated by the long electron-spin relaxation times exhibited by these systems. An alternative electron-spin based proposal exploits the large number of quantum states and the non-degenerate transitions available in individual spins. Although these advantages have stimulated vigorous research in molecular magnets, the key question of whether the intrinsic spin relaxation times are long enough has hitherto remained unanswered. Using X-band pulsed electron spin resonance, we measure the intrinsic spin-lattice ($T_1$) and phase coherence ($T_2$) relaxation rates in molecular nanomagnets for the first time. In Cr$_3$ heterometallic wheels, with $M = Ni$ and Mn, phase coherence relaxation is dominated by the coupling of the electron spin to protons within the molecule. In deuterated samples $T_2$ reaches 3 μs at low temperatures, which is several orders of magnitude longer than the spin manipulations, satisfying a prerequisite for the deployment of molecular nanomagnets in quantum information applications.

12:27PM J16.00005 Transverse magnetization and transient oscillations in the quantum tunneling of molecular magnets , TIMOTHY ZIMAN, Institut Laue Langevin/CNRS, MAXIME CLUSEL, Institut Laue Langevin — We calculate the response of a molecular magnet subject to a time-varying magnetic field and perturbatively coupled to a heat bath. The effective model of a triangle of Heisenberg spins and weak anisotropies is as has been used to model the molecular magnets $\{V_{15}\}$ and $\{Cu_{15}\}$. Oscillations parallel and transverse to the field direction correspond to transient effects in quantum tunneling. We propose that observations of these oscillations, particularly those transverse to the field, may be an effective way to probe the details of level repulsion and coupling to the environment.

12:39PM J16.00006 Energy relaxation between low lying tunnel split spin-states of the single molecule magnet Ni$_3$, G. DE LOUBENS, G. D. CHAVES-O’FLYNN, A. D. KENT, Department of Physics, NYU, C. RAMSEY, E. DEL BARCO, Physics Department, UCF, C. BEEDLE, D. N. HENDRICKSON, Department of Chemistry and Biochemistry, UCSD — We have developed integrated magnetic sensors to study quantum tunneling of magnetization (QTM) in single molecule magnet (SMMs) single crystals. These sensors incorporate a microstrip resonator (30 GHz) and a micro-Hall effect magnetometer. They have been used to investigate the relaxation rates between the 2 lowest lying tunnel split spin-states of the SMM Ni$_3$ ($S = 4$). EPR spectroscopy at 30 GHz and 0.4 K and concurrent magnetization measurements of several Ni$_3$ single crystals are presented. EPR enables measurement of the energy splitting between the 2 lowest lying superposition states as a function of the longitudinal and transverse fields. The energy relaxation rate is determined in two ways. First, in $\omega\_W$ microwave experiments the change in spin-population together with the microwave absorption directly gives the relaxation time from energy conservation in steady-state. Second, direct time-resolved measurements of the magnetization with pulsed microwave radiation have been performed. The relaxation time is found to vary by several orders of magnitude in different crystals, from a few seconds down to smaller than 100 μs. We discuss this and the form of the relaxation found for different crystals and pulse conditions.

12:51PM J16.00007 Electrodes for Molecular Spin-Valves , BRUCE HINDS, PAWAN TYAGI, STEVE HOLMES, University of Kentucky, DONGFENG LI — Realization of spin devices based on the spin-state of magnetic molecules remains a difficult challenge due to the lack of a reliable molecular electrode fabrication process. We have successfully fabricated magnetic Molecular Junctions (MJ's) by having paramagnetic molecular clusters molecules span across the surface of a metal-insulator-metal tunnel junctions (MJT) [Ta/Co/NiFe/Al$_2$O$_3$ (~2nm)/NiFe] at the exposed cross-junction pattern edge. Interestingly the current from $\sim$1μA to $\sim$1nA (RT, 100mV bias) a short time after molecular attachment presumably due to magnetic ordering. Low temperature in-plane magnetization (77 K, 0.4T) further increased magnetic ordering and decreased the junction current to $\sim$1pA level. Magnetic force microscopy (MFM) spatially showed strong antiferromagnetic coupling between the top and bottom magnetic electrodes. SQUID- magnetometer study on an array of MJT dots (4um diameter) showed reduction in magnetization after molecular attachment consistent with antiferromagnetic coupling and the dramatic changes in magneto-junction current (uA to pA).

1:03PM J16.00008 Ferromagnetism in Organic Iron Phthalocyanine Thin Films , THOMAS GREDIG, GE LIU, CORNELIU N. COLESNIIUC, IVAN K. SCHULLER, University of California, San Diego — Organic iron phthalocyanine (FePc) thin films were deposited with the planar molecule either parallel or perpendicular to the substrate. Hysteric ferromagnetic loops are observed below 5 K, lower than the previously found 15 K temperature for short range ordering in bulk powder samples. An inductive molecular magnetic anisotropy is found based on ac-susceptibility measurements with the magnetic field parallel and perpendicular to the substrate. The molecular plane spacing, as determined from X-ray diffraction, is correlated with the magnetic susceptibility. This indicates that the molecular spacing, controllable by appropriate substrate and growth temperature selection, is an important parameter for the magnetic properties of FePc. Work supported by AFOSR-MURI. [1] M. Evangelisti, J. Bartolome, L. J. de Jongh, and G. Filoti, Phys. Rev. B 66, 144410 (2002).

1:15PM J16.00009 High frequency (240 GHz) ferrimagnetic resonance (FMR) of room temperature organic based magnetic semiconductor V[TCNE]$^\_x$ (x~2) films$^1$, N.P. RAJU, The Ohio State University, K.I. POKHODNYA, The Ohio State University and University of Utah, J. IVAN TOL, NHMFL/FSU, J.S. MILLER, University of Utah, A.J. EPSTEIN — V[TCNE]$^\_x$ (x~2) is an organic based ferrimagnetic semiconducting material ($\rho_{300K}$ ~10$^{12}$cm and activation energy, $E_a$ = 0.5 eV) with an ordering temperature well above room temperature. Magnetoresistance (MR) behavior of this material has been explained on the basis of spin polarization of charge carriers in the * electronic subbands of [TCNE]$^\_x$ forming a ‘half-semiconductor’. [1,2] X-band (~9 GHz) ferrimagnetic resonance (FMR) studies on V[TCNE]$^\_x$ (x~2) have been reported earlier.[3] Temperature and angular dependence of FMR spectra of V[TCNE]$^\_x$ (x~2) films, obtained using ~240 GHz radiation, indicate the coexistence of long-range magnetic ordering and glassy behaviors. These results will be discussed in terms of competing interactions between V$^{2+}$ and [TCNE]$^\_x$ spins based on the local structural order. 1 V. N. Prigodin et. al., Adv. Mater. 14, 1230 (2002). 2 N.P. Raju et. al., J. Appl. Phys., 93, 6799 (2003). 3 S.R. Plachy et. al., Phys. Rev. B 70, 064411 (2004).

$^1$Supported by DOE grants DE-FG02-86ER45271, DE-FG02-01ER45931, and AFOSR grant FA9550-06-1-0175.
1:27PM J16.00010 Exotic quantum magnetization process observed in the \( \{ \text{Cu}_3 \} \) triangular spin ring, K.-Y. CHOI, Department of Chemistry and Biochemistry, FSU, Tallahassee, FL 32306, USA, A. P. REYES, P. L. KUHNS, NHMFL/FSU, Tallahassee, FL 32306-4380, USA, N. S. DALAL, Department of Chemistry and Biochemistry, FSU, Tallahassee, FL 32306, USA, Y. H. MATSUDA, H. NOJIRI, IMR, Tohoku University, Katahira 2-1-1, Sendai, Japan, F. HUSSAIN, U. KORTZ, School of Engineering and Science, IUB, Bremen, Germany — We present a comprehensive set of pulsed field magnetization, ESR, and NMR measurements on the triangle spin ring system \([\text{Cu}_3(\text{H}_2\text{O})_6(\alpha-\text{XW}_3\text{O}_{12})_2]^\text{2+} (X=\text{As, Sb})\). We observed half step magnetization and hysteresis loops for X=As in a fast sweeping magnetic field of \( \sim 10^4 \text{T/s} \) at 0.4 K. These features become less pronounced for X=Sb. A comparative ESR study of both compounds reveals that Dzyaloshinskii-Moriya (DM) interactions are weaker in X=Sb than X=As because of the size difference between the diamagnetic heteroatom X. This leads to a reduction of an anti-level crossing gap in X=Sb compared to X=As. This is consistent with the NMR results which show an appreciable peak of the spin-lattice relaxation rate \( 1/T_1 \) at anti-level crossing fields of 2 and 4.4 T only for X=Sb. Our work suggests that the dependence of half step magnetization on X in a nanocluster system arises from a delicate balance between the adiabatic magnetization and the relaxation rate, relying on DM interactions.

1:39PM J16.00011 Magnetic ordering and switching of iron porphyrin molecules on a substrate, OLLE ERIKSSON, Department of Physics, Uppsala University, HEIKO WENDE, Inst. fur Experimental Physik, Freie Univ. Berlin, POOJA PANCHMATIA, BIPLAL SANYAL, PETER OPPENEER, Department of Physics, Uppsala University, KLAUS BABERSCHKE, Inst. fur Experimental Physik, Freie Univ. Berlin, THEORY OF MATERIALS COLLABORATION, EXPERIMENTAL PHYSICS COLLABORATION — We have studied the structural ordering and the magnetic coupling of in-situ sublimated Fe-based porphyrin molecules on epitaxially grown Ni and Co films on Cu(100) by means of X-ray absorption spectroscopy and X-ray magnetic circular dichroism at third generation synchrotron radiation facilities, in an experimental study which is combined by density functional theory (DFT). We demonstrate the necessary sensitivity to probe the magnetic properties even for sub-monolayer porphyrin coverages. We show that due to 90 degree super-exchange interaction between Fe atoms in the molecules and atoms in the substrate (Co or Ni) the paramagnetic molecules can be made to order ferromagnetically and even have their magnetisation direction switched by a magnetisation reversal of the substrate. Theory is demonstrated to reproduce the experimental observations.

1:51PM J16.00012 Spatial and Morphology Controlled Magnetic Patterns on Organic Monolayers, SHAHID AHMAD, SALEEM RAO, DONNY MAGANA, GEOFFREY STROUSE, SHAHID SHAHEEN, Florida State University — We report on the effect of polarity of self-assembled monolayers on magnetic properties and morphology of a deposited magnetic material. Sputtering of Permalloy (Ni79Fe21) on a patterned self-assembled monolayer (SAM) structure results in formation of ferromagnetic film on polar regions and superparamagnetic clusters on non-polar regions of the SAM. These results demonstrate new opportunities for integration of controlled regions with different magnetic behavior without using conventional lithography.

2:03PM J16.00013 Magnetic ordering of new molecule-based magnet: \([	ext{Fe(TCNE)}(\text{NCMe})_2][\text{FeCl}_4]\). KONSTANTIN POKHODNYA, University of Utah/Ohio State University, MICHAEL BONNER, University of Utah, JAE-HYUK HER, PETER W. STEPHENS, Stony Brook University, ARTHUR J. EPSTEIN, Ohio State University, JOEL S. MILLER, University of Utah — The magnetic properties of \([	ext{Fe(TCNE)}(\text{NCMe})_2][\text{FeCl}_4]\) (TCNE = tetracyanoethylene), a molecule-based magnet synthesized via reaction of FeCl2(NCMe)2 with TCNE in CH2Cl2. \( M(T) \) is discussed. Both \( \chi(T) \) and \( \chi'(T) \), ac susceptibilities are almost frequency independent, and exhibit a sharp peak at \( \sim 90 \text{ K} \) in accord with ZFC and FC field cooled. The zero field cooled (ZFC) and field cooled (FC) magnetic susceptibilities, \( \chi_{ZFC}(T) \) and \( \chi_{FC}(T) \), at 5 Oe rise sharply below 95 K indicating a magnetic transition. \( \chi_{ZFC}(T) \) reaches maximum at 88 K followed by a rapid decrease suggesting an antiferromagnetic (AFM) ground state attributed to AFM coupling between ferrimagnetically ordered \([	ext{Fe(TCNE)}(\text{NCMe})_2][\text{FeCl}_4]\) layers. In contrast, \( \chi_{FC}(T) \) rises upon further cooling suggesting a strong irreversibility and indicating the presence of a remanant magnetization below 90 K, which increases upon cooling. \([	ext{Fe(TCNE)}(\text{NCMe})_2][\text{FeCl}_4]\) is the initial member of a new class of magnetic. It is the first metal-TCNE magnet with direct bonding between metal ion and [TCNE]– whose structure has been determined, and it possesses a novel planar \( \mu_2\)-[TCNE]– spin coupling unit.


11:15AM J20.00001 Substitutional NaCl hydration in ice, P. J. FEIBELMAN, Sandia National Laboratories — Na+ and Cl− can replace water molecules in ice Ih, with minimal lattice strain and without disrupting the crystal’s H-bond network. \( \text{Ab initio} \) calculations show that substitutional solvation is optimally endothermic by only 0.50 eV per NaCl formula unit. Consistent with Na+ and Cl− ionic radii of 1.0 and 1.8 Å, Na+ ions in the optimal structure lie 2.43 Å from their four equidistant, nearest O-atom neighbors, and the Cl− ions 3.02 Å from theirs. Solvation of interstitial ions is less favorable by at least 1.5 eV. These results are conclusive for molecular dynamics simulations of ionic solvation in ice; a correction for the presence of water interstitials is needed if the number of molecules in the simulation cell is chosen too large, and another for the generation of free Bjerrum defects, if anion and cation solvation are treated separately.

11:27AM J20.00002 Investigation of silicon complexes in Si-doped calcium phosphate bioceramics, P. GILLESPIE, M.J. STOTT, M. SAYER, Department of Physics, Queen’s University, Kingston, Ontario, Canada — Silicon doped calcium phosphate materials have drawn great interest as bioceramics for bone repair due to their enhanced bioactivity. However, the low level of doping in these materials, generally \儻 1 wt.%, makes it difficult to determine the effects the silicon has on the structure of these materials. In this study, silicon substituted hydroxypatite (Si-HA), silicon stabilized alpha tricalcium phosphate (Si-TCP), and a multi-phase mixture consisting of approximately 75% Si-TCP with the remainder being mainly Si-HA have been synthesized using isotypically enriched silica containing \( ^{29}\text{Si} \). \( ^{29}\text{Si} \) and charge compensation mechanisms needed to achieve this. Previous ab initio studies on these materials have investigated charge compensation mechanisms to suggest possible silicon complexes and these serve as a basis for interpreting the NMR results.

1This work is supported by the Natural Sciences and Engineering Research Council of Canada and Millenium Biologix Corp.
11:39AM J20.00003 Dose-Rate Dependence of Ionizing Radiation Damage in Silicon Transistors\textsuperscript{1}, HAROLD HJALMARSON, GEORGE VIZKELETHY, CHARLES HEMBREE, Sandia National Labs; RONALD PEASE, RLP Research. — The primary effects of ionizing radiation on silicon transistors is caused by the effects of electrons and holes created in the oxide portions of these devices. The holes can become trapped in the oxide, and they also create traps at the semiconductor-silicon interface. In the best-accepted explanation, the holes release hydrogen from source sites, often near the interface, and this hydrogen causes the interface traps by reacting with hydrogen-passivated Si dangling bonds at the interface. In this presentation, the transient electrical effects in a silicon device will be computed as a function of radiation duration, total dose, oxide defects, silicon doping and other physical variables. These calculations reveal mechanisms, such as bimolecular defect reactions, that make the damage dependent on the radiation dose rate if the total radiation dose exceeds a threshold dose.

\textsuperscript{1}Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin company, for the United States Department of Energy under contract DE-AC04-94AL85000.

11:51AM J20.00004 Information-Driven Exploration of Crystal Chemistries for Radiation Detection Materials\textsuperscript{1}, KIM FERRIS, BOBBIE-JO WEBB-ROBERTSON, Pacific Northwest National Laboratory; DUMONT JONES, Proximate Technologies, LLC. — The ability to suggest promising materials and a priori eliminate unfruitful inquiry is the key to new crystal chemistry searches. Variable spaces tend to be large and poorly defined, and property measurements (and computations) of candidate materials are not abundant. For simple binary systems, the presence of structural polymorphs and higher order compositions for A\textsubscript{m}B\textsubscript{n}; m,n=1-3 would combinatorially generate over 300,000 candidates, greatly complicating our ability to explore candidate spaces. We have used knowledge extraction methods to evolve structural signatures to direct searches using performance-based criteria. The exploratory data methods used both supervised (support-vector machines) and unsupervised (disorder-reduction and principal-component) classification methods for structural signature development. The development of new candidates for radiation detection materials will be used as the case example for this talk.

\textsuperscript{1}The authors acknowledge support from the PNNL Laboratory- Directed Research and Development Program.

12:03PM J20.00005 Electronic structure of lead pyrophosphate, MALLIGA SUEWATTANA, DAVID SINGH, Oak Ridge National Laboratory — Lead Pyrophosphate Pb\textsubscript{3}P\textsubscript{2}O\textsubscript{7} is of interest for potential radiation detection applications and use in long term waste storage. It forms in triclinic P\textsubscript{1} crystals and can also be grown as glasses. We performed electronic structure calculations using the crystal structure which determined by Mullica et. al (J. Solid State Chem (1986)) using x-ray diffraction and found large forces on atoms suggesting that the refined atomic positions were not fully correct. Here we report first principles structure relaxation and a revised crystal structure for this compound. We analyze the resulting structure using pair distribution functions and discuss the implications for the electronic properties. This work was supported by DOE NA22 and the Office of Naval Research.

12:15PM J20.00006 Full potential LAPW calculations of positron lifetimes in materials\textsuperscript{1}, HIROYUKI TAKENAKA, DAVID SINGH, Oak Ridge National Laboratory — We report positron lifetime calculations for a large number of semiconductors and insulators, including materials of interest for radiation detection. These include CdTe, ZnTe, lanthanide trihalides, orthophosphates, ZnO. Trends in lifetimes with structural features are discussed.

\textsuperscript{1}Work supported by DOE NA22.

12:27PM J20.00007 ABSTRACT HAS BEEN MOVED TO B20.00013 —

12:39PM J20.00008 Simulated electrolyte-metal interfaces – Li\textsubscript{3}PO\textsubscript{4} and Li\textsuperscript{1}, XIAO XU, YAOJUN A. DU, N.A.W. HOLZWARTH, Wake Forest U. — There has recently been a lot of interest in solid electrolyte materials such as LiPON developed at Oak Ridge National Laboratory\textsuperscript{2} for use in Li-ion batteries and other technologies. We report on the results of our model calculations on idealized interfaces between Li\textsubscript{3}PO\textsubscript{4} and Li metal, studying the structural stability and the ion mobility, using first-principles density functional techniques with the PWscf and pwpaw\textsuperscript{3} codes. Starting with a supercell constructed from Li\textsubscript{3}PO\textsubscript{4} in its crystalline γ-phase structure and several layers of Li metal, we used optimization and molecular dynamics techniques to find several meta-stable configurations. The qualitative features of the results are consistent with experimental evidence that the electrolyte is quite stable with respect to Li metal\textsuperscript{2} in addition to stability analyses, we plan to study Li-ion diffusion across the interface.

\textsuperscript{2}Supported by NSF Grants DMR-0405456 and 0427055.


12:51PM J20.00009 Li-ion diffusion mechanisms in crystalline Li\textsubscript{3}PO\textsubscript{4} electrolytes\textsuperscript{1}, YAOJUN A. DU, N.A.W. HOLZWARTH, Wake Forest University — Using first principles electronic structure methods and “nudged elastic band” optimization techniques\textsuperscript{2}, we examine ideal Li-ion diffusion in crystalline Li\textsubscript{3}PO\textsubscript{4} electrolytes, considering both vacancy and interstitialial mechanisms. The simulations are performed in supercells containing 16 Li\textsubscript{3}PO\textsubscript{4} units. We determined activation barriers for several plausible diffusion paths, considering the effects of the exchange-correlation functional forms, of the crystalline form in the β- and γ- structures, and also the effects of substitutional N. Using the generalized gradient approximation, results for γ-Li\textsubscript{3}PO\textsubscript{4} show diffusion barriers of 0.6-0.7 eV for the vacancy mechanism with a small dependence on the crystallographic direction. For the interstitial mechanism, the diffusion barriers are 0.8 eV and 1.3 eV along the b- and c-axes, respectively. The larger activation barriers of the interstitial mechanism are closer to experimental measurements on polycrystalline and single crystal samples\textsuperscript{3} which find $E_a \approx 1.1 - 1.3$ eV.

\textsuperscript{1}Supported by NSF Grants DMR-0405456 and 0427055.

\textsuperscript{2}Using the Quantum ESPRESSO package http://www.pwscf.org/.

11:03PM J20.00010 Negative-thermal-expansion ZrW₂O₉. Elasticity and pressure, CRISTIAN PANTEA, ALBERT MIGLIORI, 1, PETER LITTLEWOOD, 2, 3, YUSHENG ZHAO, HASSEL LEDBETTER, JASON LASHLEY, TSUYOSHI KIMURA, 1, JOOST VAN DJUN, 4, GLEN KOWACH, 5, LOS ALAMOS NATIONAL LABORATORY, NM TEAM, CAVENISH LABORATORY, U.CAMBRIDGE, CAMBRIDGE UK, COLLABORATION, NHMF, TALLAHASSEE, FL COLLABORATION, DEPT. PHYS.ASTRONOMY, JOHNS HOPKINS U., BALTIMORE, MD 21218, USA COLLABORATION, LUCENT TECHNOLOGIES/BELL LABS, MURRAY HILL, NJ COLLABORATION — The negative thermal expansion (NTE) compound ZrW₂O₉ is rather strange: the solid softens as its volume decreases on warming. Does ZrW₂O₉ also soften when pressure alone is applied? Using pulse-echo ultrasound in a large-volume moissanite anvil cell, we find an unusual decrease in bulk modulus with pressure at 300 K. Our results are inconsistent with conventional lattice dynamics, but a framework-solid-based non-linear model with many degrees of freedom predicts elastic softening as increases in either temperature or pressure reduce volume. The pressure-induced phase transition from α-ZrW₂O₉ (cubic) to γ-ZrW₂O₉ (orthorhombic) is found to take place at ≈ 0.5 GPa, result confirmed by Raman spectroscopy.

1:15PM J20.00011 Specific heat of tri-glycine sulfate in electric field, JASON LASHLEY, N. HUR, MIKE HUNDLEY, W. HULTS, JASON COOLEY, BOGDAN MIHALIA, JAMES SMITH, Los Alamos National Laboratory, TREVOR FINLAYSON, Monash University, CYCLONE OPERAD, CLEVELAND, OH, ROBERT RIEHN, LUKAS URBAN, ROBERT AUSTIN, Dept. of Physics, Princeton University, CHIH-KUAN TUNG, Dept. of Physics, Princeton University, — We have performed specific heat measurements on thin films of tri-glycine sulfate in an applied electric field. We find that the specific heat anomaly at T_c = 322.5 K is thermally broadened in unpoled crystals, this shape change into the characteristic λ-shape expected for a continuous transition with a 220°C electric field. The λ transition below T_c depends on T - T_c in a range T - T_c ≤ 10 K with a critical exponent, \( \beta = 0.39 \). Similarly, we find that below T_c, the experimental dielectric constant obeys an inverse-power law of the form, \( \varepsilon(T) = a/(T - T_c)^\beta \), with the constant \( a = 1244 \) K and the exponent \( \beta = 0.4 \).

1:27PM J20.00012 Effect of temperature on the thermodynamic properties of Na₂Ti₃O₇, HONG ZHANG, College of Physical Science and Technology, Sichuan University, China, HAIYING WU, Atomic and Molecular Institute, Sichuan University, China, ATOMIC AND MOLECULAR COMPUTATIONAL GROUP TEAM — The equilibrium structure of the compound Na₂Ti₃O₇ has been obtained via the minimization of the total energy within Local Density Approximation (LDA) based on Density Functional Theory (DFT), the calculated equilibrium volume are in agreement with available experimental values. In the meantime, the thermodynamic properties are investigated applying nonempirical Debye-like model combining with the first principle theory in the quasi-harmonic approximation. The evaluated equilibrium volume using this model agrees with the values from ab initio and from experiment. Our results demonstrate that this method can provide reliable predictions for the temperature dependence of these quantities such as the equation of state, the bulk modulus, the heat capacity, and the thermal expansion in detail. And our calculated thermodynamic properties are all in agreement with available experimental data.

Tuesday, March 6, 2007 11:15AM - 2:03PM — Session J27 DMP DBP: Focus Session: DNA Translocation / Nanopores - Experiments Colorado Convention Center 301

11:15AM J27.00001 A tunable DNA spring in a nanochannel, ROBERT RIEHN, RORY STAUNTON, SHUANG FANG LI, Dept. of Physics, NC State University, ROBJN BRUINSM, Department of Physics, UC Los Angeles, WALTER RESNER, Technical University of Denmark, ROBERT AUSTIN, Dept. of Physics, Princeton University — dsDNA becomes linearized when it is confined to nanofluidic channels with a cross-section of (100 nm)² or less, which has made them interesting for genomic DNA analyses. DNA is typically manipulated by means of electric fields. We have found that DNA undergoes a phase transition to a condensed state if an a.c. electric field is applied along the channel direction. The molecule collapses to about 1/4 of its initial contour length. We will discuss how the effect depends on parameters such as frequency, field strength, channel dimensions, and will discuss the origin of the effect. Interestingly, DNA behaves like an artificial muscle that can be triggered by an a.c. electric field. Since the interaction is expected to hold for any solubilized polyelectrolyte, we speculate that the mechanism may lead to a new class of polymer-based mechanical actuators. These would not suffer from depolarization like piezo transducers.

11:27AM J27.00002 dsDNA and nanobubble studies using solid-state nanopores, RALPH SMEETS, Kavli Institute of Nanoscience Delft, ULRICH KEYSER, Universitat Leipzig, DIEGO KRAPP, MENG-YUE WU, NENKE DEKKER, KAVLI INSTITUTE OF NANOSCIENCE DELFT — DNA transport through fabricated solid-state nanopores is studied at various salt concentrations. dsDNA translocation at 1 M KOCl results in a broad specific conductance profile. Contrast current pulses are observed at salt concentrations. These current changes can be understood by taking both the volume and the counter ions of the molecule into account. Nanopore conductance and noise is studied as a nanopore is moved through a laser beam. The resulting conductance profiles show strong variations in the magnitude of the conductance and the low-frequency noise. In addition, we measure an unexpected double-peak conductance profile. A nanometer-sized gaseous bubble (nanobubble) explains this profile. Our data suggest that such nanobubbles act as the dominant source of low-frequency noise and conductance variability. Currently, translocation of RecA-coated DNA is employed to detect local protein structures and test translocation models. We will report on the latest status of these experiments.

11:39AM J27.00003 Protein translocating as unfolded chains through solid-state nanopores, THOMAS AREF, ALEXEY BEZRYADIN, UIUC — We have detected translocation of the protein shrimp alkaline phosphatase (SAP) through a solid-state nanopore. The nanofluidic membrane used a highly focused electron beam in a transmission electron microscope. Once formed, the nanopore was wet with an electrolytic solution and current was driven through it by application of an electric potential. When introduced to the negative side of the nanopore, the negatively charged SAP produced current blockages as the protein molecules were driven through the pore by the electric field. No current blockages occurred when protein had not been added to the electrolytic solution nor when polarity of the applied electric field was reversed. Furthermore, this globular protein does not appear to translocate as a sphere as might be expected, but rather goes through as an unfolded chain. Our current results support a mechanism for translocation of protein molecules through solid-state nanopores. This mechanism is consistent with the constant \( \beta = 10^{-4} \text{ K}^{-1} \), and the exponent \( \epsilon = 10^{-4} \text{ K}^{-1} \). Our data suggest that such nanobubbles act as the dominant source of low-frequency noise and conductance variability. Currently, translocation of RecA-coated DNA is employed to detect local protein structures and test translocation models. We will report on the latest status of these experiments.

11:51AM J27.00004 Fabrication of sealed nanofluidic channels with single wall carbon nanotube electrodes for electronic DNA detection and analysis, CHIH-KUAN TUNG, Dept. of Physics, Princeton Univ., ROBERT RIEHN, Princeton Univ. / NC State Univ., LUKAS URBAN, Univ. of Illinois, Urbana-Champaign, ALI YAZDANI, ROBERT AUSTIN, Dept. of Physics, Princeton Univ. — Detection of entangled oligomeric polymer molecules such as DNA in nanotubes by electronic means is a challenging task. SWCNT’s are attractive nanelectrode detection elements but cannot withstand many nanofabrication techniques commonly used in making nanochannels, such as dry etching. We have used heated and temperature-programmed deposition, and create self-sealed nanochannels which plug over SWCNT’s on the substrate surface. The process is totally e-beam compatible, and therefore allows us great flexibility in addressing problems and opportunities in nanoscience electronics. We will demonstrate applications such as electronic length measurement of elongated dsDNA molecules in the sealed nanochannels.
12:03PM J27.00005 Capturing and Expulsion Processes of DNA Translocations in Solid-State Nanopores, JAMES UPLINGER, DANIEL FOLEGEA, BRIAN THOMAS, RYAN ROLLINGS, JOHN WANG, JIALI LI, University of Arkansas, Physics Department — We study the DNA translocation dynamics through voltage biased solid-state nanopores. Our study examines the capturing and expulsion process of translocation events at various conditions, and compares them to artificial events. For events with translocation time on the order of 100 µs a significant portion of the translocation event corresponds to the transitory process of the DNA entering and exiting the nanopore, which is normally included in the overall translocation time. Our study reveals that DNA enter the nanopore with a higher speed than on exit. The limitations of the electronic response of the measurement system will also be discussed.

12:15PM J27.00006 Manipulating DNA molecules inside nanopores using magnetic tweezers, HONGBO PENG, SEAN LING, Brown University — There has been intense interest recently in using solid-state nanopores for DNA sequencing. A key to this goal is to develop the capability to control the motion or translocation of DNA molecules through the pore. Magnetic tweezers provide the possibility for manipulating multiple DNA molecules through addressable nanopore arrays. We will report our experimental design as well as the preliminary results on manipulating DNA molecules inside nanopores using magnetic tweezers.

12:27PM J27.00007 Controlling DNA translocation through nanopores using optical tweezers, SHANSHAN WU, XINSHENG SEAN LING, Brown University — One of the key questions regarding DNA translocation studies is the ultimate limit to the spatial resolution of using ionic conductance measurement. We propose a method to improve on the spatial resolution by holding DNA under tension during translocation using optical tweezers. We will discuss the experimental setup and preliminary results.

12:39PM J27.00008 Metastability and capillary condensation hysteresis in nearly ideal cylindrical alumina nanopores, FELIX CASANOVA, CASEY E. CHIANG, CHANG-PENG LI, IGOR V. ROSHCIN, Physics Dept., ANNE M. RUMINSKI, MICHAEL J. SAILOR, Dept. Chemistry and Biochemistry, IVAN K. SCHULLER, Physics Dept., University of California San Diego — Nanoporous materials can be used as chemical and biological sensors. Anodized alumina, in which ordered cylindrical nanopores can be tuned in size, is a nearly ideal system to study gas adsorption and capillary condensation occurring in mesopores. Porous alumina with tunable pore diameters in the 10 to 60 nm range and a narrow distribution (<20%) were dosed with several organic vapors. Capillary evaporation occurs at equilibrium pressure for all pore sizes and gases, as predicted by the Kelvin equation. On the other hand, capillary condensation occurs within a range of metastability of the gas phase, in agreement with theoretical models. Such a hysteresis in the condensation-evaporation process is a signature of metastability and depends on the gas adsorbed. Isopropanol (with stronger surface interactions) always condenses at the same pressure, whereas for toluene (with weaker interactions), the condensation pressure is less reproducible.

1Supported by AFOSR and MEC-Fulbright.

12:51PM J27.00009 Natural Gas Storage on Nanoporous Carbon, JACOB BURRESS, MIKAEL WOOD, SARAH BARKER, JOHN FLAVIN, CINTIA LAPILLI, Dept. of Physics, University of Missouri, Columbia, MO 65211, PARAG SHAH, GALEN SUPPES, Dept. of Chem. Engineering, University of Missouri, Columbia, MO 65211, PETER PFEIFER, Dept. of Physics, University of Missouri, Columbia, MO 65211 — Powdered and monolithic activated carbons have been made that have a large methane storage capacity (Alliance for Collaborative Research in Alternative Fuel Technology, http://all-craft.missouri.edu). The current best performer stores 115-119 grams methane per liter carbon at ambient temperature and 34 bar, compared to the DOE target of 118 g/L. Results are reported for the structure of the pore space (small angle x-ray scattering, nitrogen adsorption isotherms, methane adsorption isotherms, scanning and transmission electron microscopy), the methane binding energy (methane adsorption isotherms), and computer simulations of pore formation (probabilistic cellular automata). Most pores are centered about a width of 1.1 nm. At length scales larger than 100 nm, the samples are surface fractals with fractal dimension 2.4-2.6.

1NSF (EEC-0438469), University of Missouri, Midwest Research Institute, ED (GAANN), and DOE (W-31-109-Eng-38)

1:03PM J27.00010 Structure of Alkali Metals in Silica Gel Nanopores: New Materials for Chemical Reductions and Hydrogen Production, MOUATH SHATNAWI, GIANLUCA PAGLIA, JAMES DYE, KEVIN CRAM, Michigan State University, Michael Lefenfeld, SIGNA Chemistry, SIMON BILLINGE, Michigan State University — Alkali metals and their alloys can be protected from spontaneous reaction with dry air by intercalation into the pores of silica gel (SG). The resulting powders are new convenient materials for the chemical reduction and the production of clean hydrogen. The pair distribution function was used to examine their structures. Na-K alloys added to silica gel at room temperature (stage 0) or heated to 150°C (stage I) as well as stage I Na-SG, retain the overall pattern of pure silica gel with fraction of the added alkali metals remain in the pores as nanoscale metal clusters. 2Na-MAS NMR studies confirm the presence of Na+ and demonstrate that Na+ ions are formed as well. Na-SG I when heated to 400°C (stage II) yields a dual-phase product that consists of Na2SiO3 and Na2Si2O5.

1This work was supported in part by the National Science Foundation (NSF)/CHE-0211029/, and in part by SIGNa Chemistry, LLC

1:15PM J27.00011 Anisotropy of photoluminescence from dye molecules and zeolite-dye composites, HYUNJIN LIM, HYEONSIK CHEONG, Dept. of Physics, Sogang Univ., JIN SEOK LEE, KYUNG BYUNG YOON, Dept. of Chemistry, Sogang Univ. — The dynamics of photoluminescence from dye molecules in solvents and dye-containing zeolite rods were studied using polarized photoluminescence spectroscopy. We used nanoporous zeolites and pyrrole dyes as the host and guest materials, respectively. The effects of concentration of dye molecules and zeolite-dye composites in various solvent were studied systematically. The anisotropy value (≈2.8) reached the theoretical value (≈3.0) in a highly viscous solvent (glycerol), whereas the anisotropy value is ≈1 in a low viscosity solvent (DMSO). The PL peak also shows a blue-shift in strongly polar solvents. In the case of zeolite-dye composites, we obtained a lower anisotropy value (≈2.2) in glycerol. This result is interpreted in terms of energy transfer from dye molecules inside the zeolite pores to dye molecules on the surface of zeolite crystals. We also prepared a more advanced system, dye-containing zeolite rods in uniform orientations, using pyrrole B and Y and zeolite L. The polarized PL spectra from vertically oriented monolayer of zeolite rods containing dye molecules show that the anisotropy ratio is ≈9 when the polarization direction of excitation light and the c-axis of zeolite rods are parallel.
**1:27PM J27.00012 How conductive polymer/nano-conductive filler composites can be?**  
SUPING LYU, DARREL UNTEREKER, JAMES SCHLEY, Medtronic Corporate Science and Technology — How conductive can polymer/filler composites be? It was thought the conductivity of composites could be increased by reducing the sizes of the fillers or increasing their aspect ratios, for example, by using carbon nanotubes. Invention of numerous conductive nanomaterials provides opportunity to verify this idea and to achieve higher conductivity. However, the highest conductivity of composites achieved was just a few percent of that of bulk materials of the fillers, regardless whether the filler was silver micron particles, platinum nano particles, carbon nano particles, or carbon nano tubes. The conductivity of filler-based composite is intrinsically limited by the micro-contact between the conductive fillers. Reducing the filler size or increasing aspect ratio did not yield significant improvements in conductivity although percolation may occur earlier.

**1:39PM J27.00013 Free-volume anomaly in confined glycerol.**  
DUNCAN KILBURN, Indiana University Cyclotron Facility, VICTORIA GARCIA-SAKAI, NIST Center for Neutron Research and University of Maryland, ASHRAF ALAM, Bristol University, PAUL SOKOL, Indiana University Cyclotron Facility — Glycerol is a small molecule glass-former which exhibits relatively high viscosity due to its extensive hydrogen bonding. Here we report the first measurements of local free volume and local mobility of glycerol confined in Vycor: a mesoporous silica glass with pores 70 Angstroms in diameter. We find that the lower molecular mobility in confinement (measured here using quasi-elastic neutron scattering) is accompanied by a higher mean free-volume size between molecules (as measured using positron annihilation lifetime spectroscopy). The strong wetting between glycerol and the glass surface appears to perturb the glycerol to such an extent that the normally observed free-volume/mobility relationship is reversed. Previous studies have come to similar conclusions (high glass transition temperature, low density) but this is the first to show that these effects originate locally. This is expected to have significant ramifications for the study of hydrogen-bonding liquids in confinement, for example water — a topic of much current interest due to its application in hydration water in biological material.

**1:51PM J27.00014 Induced Thermal Dynamics in Aerosil Dispersed Glass Forming Liquid.**  
DIPTI SHARMA, GERMANO IANNACCHIONE, Worcester Polytechnic Institute — A high-resolution calorimetric spectroscopy study has been performed on pure glycerol and colloidal dispersions of an aerosil gel in glycerol covering a wide range of temperatures from 30 to 300 K, deep in the liquid phase of glycerol. The colloidal glycerol-aerosil samples with 0.07, 0.14, and 0.32 grams of silica per cm$^3$ of glycerol reveal activated energy (thermal) dynamics at temperatures well above the $T_g$ of the pure glycerol. The onset of these dynamics appears to be due to the frustration or pinning imposed by the silica gel on the glycerol liquid. Since this behavior occurs at relatively low silica density (large mean-void length compared to the size of a glycerol molecule), this induced dynamics is likely due to a cooperative mode of glycerol molecules with the aerosil gel via mutual hydrogen-bonding. However, the exact nature of these energy dynamics is not known. The study of such frustrated colloids may provide a unique avenue for illuminating the physics of glasses.

---

**Tuesday, March 6, 2007 11:15AM - 2:15PM**  
Session J28 DMP: Focus Session: Carbon Nanotube Optics III  
Colorado Convention Center 302

**11:15AM J28.00001 Resonance Raman of Single-Wall Carbon Nanotubes**  
ADO JORIO, Universidade Federal de Minas Gerais — The use of resonance Raman spectroscopy to study and characterize single-wall carbon nanotubes (SWNTs) will be discussed. The achievements and limitations of the technique for metrology purposes will be presented, addressing the importance of the excitonic nature of the optical transitions. We use the method to understand the effect of carbon nanotube doping. The efforts to extend the Kataura plot to larger tube diameters and higher optical transitions not only extend our characterization capability, but also sheds light into the nature of the optically active levels. Experimental results that have not been predicted by solid state approaches are understood on the basis of quantum chemical calculations. It is also interesting to discuss some results on nano-ribbons and their relations to carbon nanotubes.

1Support from Kavli Foundation and CNPq, Brazil.

**11:51AM J28.00002 Raman Studies of Exciton-Phonon Coupling in Carbon Nanotubes: Quan-titation of Bundled vs. Isolated Behavior.**  
STEPHEN DOORN, ANDREW SHREVE, SERGEI TRETIAK, Los Alamos National Laboratory, ZHENGTANG LUO, FOTIOS PAPADIMITRAKOPOULOS, University of Connecticut — Exciton-phonon and electron-phonon coupling are important for a number of carbon nanotube optical and transport behaviors and have recently drawn attention for their role in chirality-dependent optical properties observed in radial breathing mode (RBM) Raman spectra. Given the importance of these effects, there is a need to quantitate the magnitude of the exciton-phonon coupling. We present a new analysis of Raman absorption of RBM fundamental and overtone intensities that transfer the magnitude of coupling for five specific nanotube chiralities. These results agree with values predicted through quantum chemical calculations and indicate that non-Condor effects may be important in describing nanotube transitions. We extend the analysis of the coupling to bundled nanotube samples and find it decreases significantly in these sample types. We also discuss the coupling behavior of a new class of intermediate frequency modes (IFMs) that display step-wise dispersive behavior. These IFMs are associated with coupling between the E11 and E22 transitions. Bundling is found to increase the coupling observed for these modes.

**12:03PM J28.00003 Exciton-phonon interaction and Raman intensity of carbon nanotubes**  
RICHIRO SAITO, Tohoku University, CREST JST, JIE JIANG, Dept. of Phys. NC State Univ., ADO JORIO, Dept. of Phys., TOHOKU UNIVERSITY, KENTARO SATO, Dept. of Phys. Tohoku Univ., GENE DRESSELHAUS, MILLIE DRESSELHAUS, MIT — Using extended tight binding framework, the exciton states and exciton-phonon interaction are calculated for understanding optical properties of single wall carbon nanotubes. Resonance Raman intensity for first and second-order, intervalley, resonance Raman processes. Although the exciton-phonon interaction is not so different from the electron-phonon interaction, the optical absorption (emission) is enhanced significantly by the localized exciton wavefunctions. References: J. Jiang et al, Phys. Rev. B, in press.

2RS acknowledges MEXT grant (No. 16076201)

**12:15PM J28.00004 Tunable Electron-phonon Coupling in Isolated Metallic Carbon Nanotubes Observed by Raman Scattering.**  
YANG WU, JANINA MAULTZSCH, Columbia University, ERNST KNOESEL, Rowan University, BHUPESH CHANDRA, Columbia University, MINGYUAN HUANG, Columbia University, MATT SFEIR, Columbia University, LOUIS BRUS, JAMES HONE, TONY HEINZ, Columbia University — Metallic single-walled carbon nanotubes can exhibit significant broadening of the high-energy (G) mode Raman features. In contrast to narrow Raman widths for semiconducting nanotubes, full widths in excess of 50/30 are commonly observed in metallic nanotubes. Different possible physical origins have been proposed in previous literatures. In this paper, we demonstrate the ability to modify the Raman linewidth by electrostatic gating. Using measurements of individual suspended nanotubes, we find that either a positive or negative shift in the Fermi energy by an applied electrostatic field can reduce the linewidth by more than a factor of two. The results can be understood in terms of blocking vertical electronic transitions (electron-hole pair generation) possible for the zone-center phonons in an unperturbed nanotube, but not in a nanotube with a sufficiently shifted Fermi level. A simple model is presented to explain the experimental results.
12:27PM J28.00005 Ultrafast Spectroscopy of Phonons in Single-Walled Carbon Nanotubes. ERIK HAROZ, Rice University, DAVID HILTON, JUNICHIRO KONO, RÓBERT HAUGE, Rice University, KI-JU YEE, Chungnam National University, YONG-SIK LIM, Konkuk University, STEPHEN DOORN, Los Alamos National University — Recently, we observed coherent phonons (CPs) of the radial breathing mode (RBMs) in semiconducting single-walled carbon nanotubes (SWNTs) suspended as individuals in aqueous surfactant (1). We demonstrated CP spectroscopy as a powerful method for determining phonon and exciton energies in an ensemble of SWNTs with different chiralities. Here, we extend this ultrafast optical studies on various types of nanotube samples including films and solutions. In order to provide new insight into CP decay mechanisms, we systematically investigated the temperature dependence of CP amplitude, frequency, and lifetime from 4 -300 K while changing the pump/probe photon energy. We also investigated how bundling affects CP line widths. Furthermore, we compared the intensity dependence of CPs resonant with the $E_{11}$ and $E_{22}$ transitions by studying the excitation profile for specific RBMs, focusing particularly on the excitation line width and shape. 1) Y. S. Lim et al., Nano Letters, published electronically November 2, 2006.

12:39PM J28.00006 Theory of coherent phonons in carbon nanotubes1. GARY SANDERS, CHRIS STANTON, University of Florida — We develop a general theory for the generation of coherent phonons in single wall carbon nanotubes or arbitrary chirality. Coherent phonons are generated in the nanotube via the deformation potential electron-phonon interaction with photogenerated carriers. In our theory the electronic states are treated in a third nearest neighbor tight binding formalism which gives a good description of the states over the entire nanotube Brillouin zone while the nanotube phonon states are treated in a valence force field model that includes bond-stretching, in-plane and out-of-plane bond-bending, and bond-twisting interactions. In the tight-binding electron-phonon interaction, all two center integrals out to fourth nearest neighbors are retained. The equations of motion for the coherent phonon amplitudes are obtained in a density matrix formalism and we find that the coherent phonon amplitudes satisfy driven oscillator equations for each value of the phonon wavevector. We will discuss excitation strengths for different coherent phonon modes and compare to recent experiments.

1Supported by NSF DMR-0325474

12:51PM J28.00007 Intrinsic BWF-lineshape Observed by Raman Scattering in Isolated Metallic Carbon Nanotubes. JANINA MAULTZSCH, YANG WU, Columbia University, ERNST KNOESEL, Rowan University, BHUPESH CHANDRA, MINGYUAN HUANG, MATT SFEIR, LOUIS BRUS, JAMES HONE, TONY HEINZ, Columbia University — Broadened and asymmetric lineshapes for Raman scattering in the high-energy (or G) modes of metallic carbon nanotubes have been reported for many years. There remains, however, controversy about whether this behavior is an intrinsic feature of metallic nanotubes or is induced by perturbations. To address this issue, we have examined isolated metallic nanotubes suspended in air, with chiral indices determined independently by Rayleigh scattering and Raman measurements of the radial breathing mode. Our data show that strong broadening (to FWHM > 50/cm) and weak asymmetry are typical of the high-energy Raman modes, with lineshapes describable by a Breit-Wigner-Fano (BWF) form. Significant variation in peak width and Raman shift is, however, observed as a function of the nanotube chiral index. Indeed, some metallic nanotubes have lineshapes and widths that are very similar to those of semiconducting nanotubes. We will discuss the observed variation and the origin of the BWF lineshape.

1:03PM J28.00008 Bundling and Electronic Effects on the BWF Feature for Doped and Undoped Carbon Single-wall Nanotubes. JEFF BLACKBURN, TIMOTHY MCDONALD, CHAIWAT ENGTRAKUL, ANNE DILLON, MICHAEL HEBEN, National Renewable Energy Laboratory — In this contribution we examine the role of bundling and electronic effects on the Breit-Wigner-Fano (BWF) Raman component for dispersions of undoped and boron-doped (p-type) SWNTs in various surfactants. Interestingly, we find that the intensity of the BWF component is sensitive to the degree of SWNT debundling, solution pH, doping level, charge transfer with redox active molecules, and differences in the SWNT-surfactant interactions, all of which lead to varying degrees of charge localization at the nanotube surface. In several cases, we observe a strong BWF component in the metallic Raman spectrum even for dispersions of highly isolated SWNTs. In general, our results, coupled with results from the literature, suggest that the presence and intensity of the BWF feature is sensitive to any changes in the magnitude of dielectric screening, whether from tube-tube interactions in bundles, from charge injection or depletion, or from charge polarization from tube-molecule interactions. These results suggest that, contrary to practice in some recent studies, the existence or lack of a BWF feature should not be used alone as a measure of SWNT aggregation. They also provide information regarding the nature of surfactant-nanotube interactions, SWNT redox chemistry, and nanotube separations.

1:15PM J28.00009 First-principles study of resonant Raman spectroscopy in graphite and carbon nanotubes1. DAVID PRENDERGAST, University of California at Berkeley and Lawrence Berkeley National Laboratory, JACK DESLIPPE, University of California at Berkeley, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — Resonant Raman spectroscopy is an increasingly used experimental tool for the characterization of carbon nanotubes (CNTs). It explores the coupling of optical, electronic, and vibrational modes in these quasi-one-dimensional systems. Using first-principles methods we calculate the electron-photon and -phonon matrix elements necessary to estimate the first-order Raman cross-section. For graphite, the non-interacting quasiparticle spectrum is sufficient, however, for CNTs, the excitonic spectrum and wave functions require an accurate description of electron-hole correlation. We calculate excitonic effects by solving the Bethe-Salpeter equation, using as input the quasiparticle spectrum obtained within the GW approximation to the electron self-energy. We analyze the exciton-photon coupling in CNTs and its impact on the resonant Raman cross-section.

1This work was supported by National Science Foundation Grant No. DMR04-39768, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and SDSC.

1:27PM J28.00010 Signature of the electron-phonon interaction in the electron spectral function of graphene. CHEOL HWAN PARK, FELICIANO GIUSTINO, MARVIN L. COHEN, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — The spectral function of graphene has been measured with high energy and momentum resolution by angle-resolved photoelectron spectroscopy. It has been proposed that the measured spectral function exhibits combined signatures from electron-photon, electron-electron, and electron-plasmon interactions. We here present a first-principle investigation of the contribution to the electron self-energy of graphene arising from the electron-phonon interaction. We compute the electron self-energy treating the graphene bandstructure within density functional theory, the lattice dynamics within density functional perturbation theory, and the electron-phonon interaction within the Migdal approximation. Due to its peculiar cone-shaped bandstructure, the electron-phonon contribution to the electron self-energy of graphene shows qualitative differences as compared to the case of ordinary bulk metals.

1This work was supported by the NSF under Grant No. DMR04-39768, and the U.S. DOE under Contract No. DE-AC02-05CH11231. Computer time was provided by NERSC and NPACI.
1:39PM J28.00011 1st and 2nd order Raman scattering from n-Graphene Layer (nGL) Films on Silicon Substrates. , AWNISH GUPTA, GUGANG CHEN, PETER EKLUND, Department of Physics, The Pennsylvania State University — Results of room temperature Raman scattering experiments on graphene and n-graphene layer films (nGLs) will be presented [1]. We find that the G band at ~1582 cm⁻¹ exhibits an interesting upshift in frequency with 1/n which we tentatively assign to a surface strain phenomenon connected with surface roughness of the substrate and compensated by the increase in stiffness of the nGL with increasing n. Interesting n-specific bands are observed in the ~1350 cm⁻¹ (or D-band) region which may correlate with deviations from planarity of the nGL. The second order scattering is very interesting and for small n (n<4) the (2D' or G') band intensity at ~2700 cm⁻¹ is actually higher than the first-order G-band scattering. The shape of this band is sensitive to n and thus can be used to identify n without an AFM measurement. Whereas, the 2D' band is sensitive to n, the 2nd order 2G band ~3248 cm⁻¹ is independent of n. These observations will be discussed in terms of the phonon and electronic dispersion of nGLs. 1. A. Gupta, G. Chen, P. Joshi, S. Tadigadapa and P.C. Eklund, “Raman Scattering from High-Frequency Phonons in Supported n-Graphene Layer Films” NanoLett (in Press).

1:51PM J28.00012 Raman Scattering Study of the Graphene-Substrate Interaction. , PETER EKLUND, AWNISH GUPTA, GUGANG CHEN, Department of Physics, The Pennsylvania State University — We report on Raman scattering studies of graphene and few graphene layer films (i.e., nGLs, where n is the number of graphene layers in the film). nGL films (n=1-3, 25) were prepared by mechanical transfer from HOPG to various substrates (SiO2:Si, Au, Ag, cleaved Mica, and free-standing films). For metallic substrates we observed a clear G-band frequency downshift relative to that observed when the nGL is on SiO2:Si. This downshift is interpreted in terms of a chemical charge transfer of electrons from the metallic substrate to the nGL. Interestingly, the position and shape of the 2D' (or G') band at ~2700 cm⁻¹ is found insensitive to the substrate interaction.

2:03PM J28.00013 Raman Spectroscopy of single and double layer graphene, YAN YIN, SEBASTIAN REMI, SVELTANA ANISSIMOVA, ANNA SWAN, BENNETT GOLDBERG, Boston University — Dirac fermions and novel quantum Hall effects. Graphene also holds the promise of one day replacing silicon in microchips. Early Raman scattering has identified basic features of the G-band and D-band, where the former shows intensity dependence associated with addition of single layers, and the latter displays significant intensity only for the single and double layer systems. We have performed room-temperature Raman scattering with a spatial resolution of 0.5 microns consistent with this work. More recently, Pinczuk and Kim and co-workers have shown low-temperature Raman scattering that displays evidence of electron density dependent screening. We investigate the interlayer hopping with temperature-dependent Raman scattering and in our low-temperature Raman, we specifically investigate the novel coupling and edge states predicted by Castro Neto and co-workers.
12:15PM J39.00004 Hydrogen molecule binding to unsaturated metal sites in metal-organic frameworks studied by neutron powder diffraction and inelastic neutron scattering

YUN LIU, NIST Center for Neutron Research; Dept. of Material Science and Engr., Univ. of Maryland, College Park, CRAIG BROWN, NIST Center for Neutron Research; Indiana Univ. Cyclotron Facility, DAN NEUMANN, NIST Center for Neutron Research, MIRCEA DINCA, JEFFREY LONG, Dept. of Chemistry, Univ. of California, Berkeley, VANESSA PETERSON, CAMERON KEPERT, School of Chemistry. The Univ. of Sydney — Metal organic framework (MOF) materials have shown considerable potential for hydrogen storage arising from very large surface areas. However, the low binding energy of hydrogen molecules limits its storage capability to very low temperatures (< 77 K), which is impractical for industrial applications. Using neutron powder diffraction (NPD), we have characterized the hydrogen adsorption properties in a variety of unsaturated metal ions. Direct binding between the unsaturated metal ions and hydrogen molecules is observed and responsible for the enhanced initial hydrogen adsorption enthalpy. The different metals centers in these MOFs show different binding strength and interaction distances between the hydrogen molecule and metal ions. The organic linker also affects the overall H2 binding strengths. Inelastic neutron scattering spectra of H2 in these MOFs are also discussed.

1We acknowledge the support of the Petroleum Research Fund and Research Corporation

12:27PM J39.00005 Infrared spectroscopy of trapped hydrogen in metal-organic-frameworks

STEPHEN FITZGERALD, KELTY ALLEN, PATRICK LANDERMAN, JESSE ROWSELL, Oberlin College — We present a novel use of diffuse reflectance infrared spectroscopy to study the quantum dynamics of molecular hydrogen trapped within metal-organic-framework (MOF) hosts. This technique is particularly useful in the context of hydrogen storage since it provides detailed information about the intermolecular potential at the binding site. The spectra consist of quite sharp bands associated with the quantized vibrational and rotational motion of the trapped hydrogen. The vibrational bands are redshifted relative to the gas phase while the rotational sidebands contain an additional fine structure due to the orientational dependence of the binding potential. Results on MOF-5 reveal the presence of two primary binding sites. The first saturates at a loading concentration on the order of 4 H2 per Zn ion and has a binding energy of roughly 4 kJ/mole. The second has a somewhat lower binding energy. Both sites produce an ortho to para conversion rate on the order of 30-50 % per hour.


KATHLEEN LASK, VAIVA KRUNGLEVICIUTE, ALDO MIGONE, Department of Physics, Southern Illinois University Carbondale, J.-Y. LEE, JING LI, Department of Chemistry and Chemical Biology, Rutgers University — We have measured the adsorption kinetics of two gases, freon and argon, on two microporous metal-organic framework materials, RPM-1 (or [Cu2(bpc)2(H2O)2]·4DMF·H2O, bpc = biphenyldicarboxylate) and Cu-BTC (or [Cu4(btc)2(H2O)2]), btc = benzenetricarbocylexate). The measurements were conducted at comparable values of the scaled temperatures (Tisothers/Tcritical) for the respective gases. In our experiments, we monitor the pressure decrease as a function of time after a dose of gas is admitted into the experimental cell. The kinetics results obtained for both gases are similar on Cu-BTC, while they are significantly different in RPM-1. Our results indicate that RPM-1 has potential for gas separation for mixtures of species with dimensions similar to argon and freon; this is not the case for Cu-BTC MOF.

12:51PM J39.00007 ABSTRACT WITHDRAWN
1:39PM J39.00011 In-situ electronic structure study of H₂ adsorption on HOPG  
PER-ANDERS GLANS, JINGHUA GUO, ALS, Lawrence Berkeley National Laboratory — The storage of hydrogen in a both safe and compact manner is of great importance for, for example, hydrogen powered vehicles. Interesting candidates for dense storage of hydrogen are different types of carbon based nanomaterials: single (SWCNT) and multi-walled carbon nanotubes, C₆₀ and C₇₀. Various groups have reported different amounts of hydrogen stored using SWCNTs. Highly ordered pyrolytic graphite (HOPG) has similarities with the carbon systems mentioned above. Photon-in, photon-out techniques are well suited for measurements of the electronic structure of these materials under ambient hydrogen pressure. X-ray absorption (XAS) and emission spectroscopy (XES) measurements have been performed on HOPG under different hydrogen pressures. The measured partial density of states of this system will be presented.

1:51PM J39.00012 Hydrogen Adsorption on Nanoporous Biocarbon¹  
M.B. WOOD, J.W. BURRESS, C.M. LAPILLI, P. PFEIFER, Dept. of Physics, University of Missouri, Columbia, MO 65211, P.S. SHAH, G.J. SUPPES, Dept. of Chemical Engineering, University of Missouri, Columbia, MO 65211, A.C. DILLON, P.A. PARILLA, National Renewable Energy Laboratory, Golden, CO 80401 — As a part of the Alliance for Collaborative Research in Alternative Fuel Technology (http://all-craft.missouri.edu) we study activated carbons made from corncob, optimized for storing methane and hydrogen (H₂) by physisorption at low pressure. We report here: (a) storage capacities of 73-91 g H2/kg carbon at 77 K and 47 bar, validated in three different laboratories (the 2010 DOE target is 60 g H2/kg system); (b) binding energies from H₂ adsorption isotherms (c) temperature-programmed desorption data; (d) degree of graphitization of the carbon surface from Raman spectra; (e) pore structure of carbon from nitrogen and methane adsorption isotherms, and small-angle x-ray scattering. The structural analysis shows that the carbon is highly microporous and that the pore space is highly correlated (micropores do not scatter independently).

¹NSF (EEC-0438469), University of Missouri, Midwest Research Institute, ED (GAANN), and DOE (W-31-109-Eng-38)

2:03PM J39.00013 Adsorption of supercritical carbon dioxide and propane in porous aerogel.  
YURI MELNICHENKO, GERNOT ROTHER, GEORGE WIGNALL, Neutron Scattering Sciences Division, ORNL, Oak Ridge, TN 37831, USA, DAVID COLE, Chemical Sciences Division, ORNL, Oak Ridge, TN 37831, USA, HENRICH FRIELINGHAUS, Forschungszentrum Julich, IFF, D-52425, Germany — We demonstrate that small-angle neutron scattering (SANS) can be used to determine the density and volume fraction of the adsorbed fluid phase in porous materials. The developed methodology is used to study the adsorption of near-critical CO₂ and propane in aerogel as a function of pressure and temperature. For the first time the variation of the density and volume fraction of the adsorbed phase of near-critical fluids is reported and analyzed. These parameters are used to determine the absolute fluid adsorption without additional assumptions commonly used in the literature. The adsorption of CO₂ and propane (8 g/g and 1 g/g, respectively) is found to be significantly higher in aerogels than in activated carbons and silica gels. The results provide new insights in the adsorption behavior of supercritical fluids, such as a non-monotonic variation of the density of the adsorbed phase and depletion of aerogel at high pressures.

Tuesday, March 6, 2007 11:15AM - 1:51PM —  
Session J42 DMP: Focus Session: Metal-Semiconductor Interfaces  
Colorado Convention Center 505

11:15AM J42.00001 Shape transition and migration of TiSi₂ nanostructures embedded in a Si matrix.  
ANDERSON SUNDA-MEYA, Department of Physics, North Carolina State University, DAVID J. SMITH, Department of Physics, Arizona State University, ROBERT J. NEMANICH, Department of Physics, North Carolina State University — While the embedding of epitaxial nanostructures, like SiGe, on Si surfaces does not affect their epitaxial position on the substrate, this study establishes that under conditions of epitaxial Si deposition, TiSi₂ nanostructures undergo a shape transition and “migrate” to the surface. They were grown on a Si[001] surface by depositing 0.5 nm of Ti at 750 °C and annealing for 2 min. They were then buried under a Si capping layer at different temperatures and thicknesses. AFM and XREM have been used to study their shape, geometry and evolution. Many of the buried structures were found to display a near uniform hemispherical shape. Their density and size were observed to be temperature dependent. The buried islands induce inhomogeneous stress profiles on the capping layer surface. The AFM images of the islands showed square holes at the surface aligned along the [110] directions suggesting that the Si layer was terminated along {111} planes. Many islands displayed faceting observed in cross-sectional electron micrographs. The observed structural changes are rationalized in terms of the interplay between thermodynamics and kinetics, solid state capillarity, and the roughening transition.

11:27AM J42.00002 Growth and stability of dysprosium silicide nanostructures on Si[001]  
MATTHEW ZEMAN, ROBERT NEMANICH, North Carolina State University — The growth and coarsening dynamics of epitaxial dysprosium silicide nanostructures on Si[001] are observed using tunable ultra-violet free electron laser excitation for photo-electron emission microscopy (PEEM). A dense array of compact silicide nanostructures is observed to coarsen during annealing at 950-1050°C. Some of the nanostructures grow into large flat-topped rectangular islands at the expense of smaller islands which disappear via Ostwald ripening. The coarsening rate of the island distribution increases with increasing temperature, and the formation of a flat top on the growing islands is related to strain relaxation. Additionally, the shape and growth rates of the islands may be influenced by the island crystal structure and/or local island distributions. A subsequent deposition of dysprosium onto the surface results in the nucleation of new island and the formation of a flat top on the growing islands is related to strain relaxation. Additionally, the shape and growth rates of the islands may be influenced by the island crystal structure and/or local island distributions. A subsequent deposition of dysprosium onto the surface results in the nucleation of new island and nanowire structures. Immediately after the deposition is terminated the nanowires begin to decay from the ends while the larger island structures grow. The decay of the wires can be attributed to Ostwald ripening and is explained in terms of the Gibbs-Thompson relation, where the high adatom concentration at the nanowire ends leads to the diffusion of adatoms away from the wires towards the larger surrounding structures. In situ movies will be presented which detail the growth and coarsening processes.

11:39AM J42.00003 Spatial First-passage Statistics of Al/Si(111)-(√3 × √3) Step Fluctuations: Implications for Nanoscale Structures¹  
BRAD CONRAD, WILLIAM CULLEN, University of Maryland, DANIEL DOUGHERTY, NIST, IGOR LYUBINETSKY, PNNL, ELLEN WILLIAMS, University of Maryland — The step-edges on a multi-component surface of Al/Si(111)-(√3 × √3) observed via scanning tunneling microscopy, fluctuate in thermal equilibrium over a temperature range of 720K-1070K. For step lengths L = 65-160 nm, the measured first-passage spatial persistence and survival probabilities are found to be temperature independent and thus universally applicable. The power-law functional form for spatial persistence probabilities is confirmed, and the symmetric spatial persistence exponent is measured to be θ = 0.53±0.05, in agreement with the theoretical prediction θ = 1/2. The survival probability is found to scale with y/L, where y is the distance along the step edge. The functional form of the survival probabilities agrees quantitatively with the theoretical prediction, which decays exponentially as exp(-y/y₀) for small y/L. The experiment finds the decay constant to be y₀/L = 0.076 ± 0.033 for y/L ≤ 0.2. The physical implications of these results for the predictability of nanoscale displacements and thus on device design and manufacturing will be discussed.

¹Supported by the UMD NSF-MRSEC under grant DMR 05-20471. The NSF-MRSEC SEF was used in obtaining the data presented.
11:51AM J42.00040 Au-Induced Nanostructuring of Vicinal Si Surfaces — MARK GALLAGHER, WEI WU, LAURA PEDRI, Lakehead University — The deposition of extremely small amounts of metal onto vicinal semiconductor surfaces can cause dramatic changes in morphology on a nanometer scale. This recent has been exploited to self-assemble arrays of atomic chains that exhibit bands with intriguing one-dimensional (1-d) metallic behavior. Depositing Au onto a vicinal Si(111) sample tilted either towards or away from the [112] can produce an array of 1-d chains running along the [110] direction. To investigate the nanofaceting underlying chain formation, we have measured the surface morphology of several miscuts as a function of Au coverage using scanning tunneling microscopy. Samples oriented 3.8°, 8°, and 12.5° from [111] towards [112] have been measured with Au coverages ranging from less than 0.06 ML up to 0.5 ML. All surfaces exhibit nanofacets with orientations that depend critically on Au coverage. On the 8° sample, while the exact nature of the surface morphology depends on Au coverage, below 0.32 ML all surfaces incorporate (775)-Au nanofacets. Similarly, (775)-Au facets are also observed on the 3.8° sample. At 0.17 ML the surface consists of (111)×7×7 and (775)-Au nanofacets. At 0.4 ML the (111) terraces transform from 7×7 to a 5×2, and the surface consists of (111)×5×2–Au terraces separated by (775)-Au facets. The persistence of the (775)-Au facet reinforces the idea that it represents a low energy facet on these Au modified vicinal surfaces.

12:03PM J42.00055 Density Functional Study on Energetic Instability of the 5×2 structure on Au/Si(111) and Au/Si(775) surfaces — MASASHI NODA, TAKUYA KADOHIRA, SATOSHI WATANABE, Dept. of Materials Engineering, The University of Tokyo and CREST-JST, CHRIS FISCHER, GERBRAND CEDER, DMSE, Massachusetts Institute of Technology — Atomic configurations of Au/Si(111) surface have been examined extensively. However, there are only few systematic theoretical analyses taking account of the variation of Au and Si coverages. Keeping this in minds, we have done such a systematic analysis on the energetic stability of various models proposed for Au/Si (111) structures so far using density functional calculations. As a result, we obtained good agreement with experimental results on the periodicity of energetically stable structures except that none of the models with 5×2 periodicity are predicted to appear in our calculation. Then, we examined the possibility of realizing some of the 5×2 models by the effects of steps, using Au/Si(775). We found that none of the 5×2 structures are stable even on Si(775). These results suggest that we have to explore a new model to explain the observed 5×2 structure.

12:15PM J42.00066 One-dimensional plasmons in atom wires on Si(111)-5x2-Au — T. NAGAO, C. LIU, S. YAGINUMA, T. NAKAYAMA, National Institute for Materials Science — One-dimensional (1D) collective excitation in atom wires self-assembled on the Si(111)-5x2-Au surface is investigated. Electron scattering spectroscopy using highly collimated slow electron beam has detected a characteristic sound wave-like excitation that exhibits strong anisotropy along the wires. This excitation occurs in dipole scattering regime and its lifetime drops as a function of momentum. From these features, the observed loss is assigned to a unique plasmon mode confined in the atom wires which are revealed to be strongly metallic.

12:27PM J42.00077 First-principles calculations of low coverage growth of Ba on Si(001) — C. R. ASHMAN, High Performance Technologies Inc., C. J. FOERST, P. E. BLOECHL, Clausthal University of Technology, DOD HPCMP PET PROGRAM COLLABORATION, CLAUSTHAL UNIVERSITY OF TECHNOLOGY, INSTITUTE FOR THEORETICAL PHYSICS COLLABORATION — Ba is of interest to the semiconductor industry for it’s possible use in replacement gate oxide materials and for possible use in a buffer layer between Si(001) and Ba containing dielectric materials. Thus it is of importance to understand the initial stages of growth. This paper reports state-of-the-art electronic structure calculations on the deposition of Barium on the technologically relevant, (001) oriented silicon surface. We identify the surface reconstructions from zero to one monolayer and relate them to previous theoretical studies of low coverage Ba growth and Sr growth.

12:39PM J42.00088 Controlled self-organization of atomic vacancies in pseudomorphic adsorbate layers: Ga/Si(112) — E.J. MOON, University of Tennessee, Knoxville, USA, P.C. SNUJDERS, Kavli Institute of Nanoscience, Delft, The Netherlands, C. GONZÁLEZ, J. ORTEGA, F. FLORES, Universidad Autónoma, Madrid, Spain, H.H. WEITERING, University of Tennessee, Knoxville, and Oak Ridge National Laboratory — Ga adatoms on Si(112) result in the formation of pseudomorphic Ga chains. Compressive strain in these atom chains is effectively released via the creation of adatom vacancies and their self-organization into almost evenly spaced vacancy lines (VL). Here, we present a detailed study of these line defects using scanning tunneling microscopy, low energy electron diffraction, and density functional theory calculations. The average spacing between line defects can be varied continuously, within limits, by adjusting a single control parameter: the chemical potential of the Ga adatoms. The bulk resistivity at room temperature is close to the reported value, indicating a scattering mechanism which is mixture of both skew scattering and side jump scattering. 1. K. Fuchs, Proc. Camb. Phil. Soc. 34, 100 (1938)
1:15PM J42.00011 Interfacial Structure of Fe-GaAs(001) with annealing and substrate surface morphology. RYAN PHILIP, JONG-WOO KIM, Ames Laboratory, PAUL MICELLI, University of Columbia-Missouri, JUSTIN SHAW, National Institute of Standards and Technology, CHARLES M. FALCO, University of Arizona — The primary obstacle confronting ‘spintronics’ is the inability to efficiently create a single spin resolved current within a semiconductor. There are two leading approaches, create a magnetic semiconductor with a Tc above room temperature, as yet elusive and the ability to inject a spin current from a transition metal film into a semiconductor. The issue at hand in the latter is the ‘spin scattering’ interface between the overlayer and substrate. This has led to many studies to understand the magnetic evolution of very thin transition metal films on semiconductor substrates, notably Fe on GaAs. Here we will report on the recent and ongoing high flux grazing X-Ray diffraction studies of in-situ grown Fe films on prepared GaAs(001) surfaces at the Advanced Photon Source. Extended specularity diffraction data has been fit with kinematic calculations to model the vertical structure of the film and interface. In plane grazing diffraction investigates the in-plane relaxation process. This data has been coupled with pregrown Al capped Fe films also on GaAs(001) prepared at University of Arizona. The films have been annealed at incremental temperatures and have been studied with BLS in order to correlate the magnetic in-plane anisotropic nature with the in-plane film strain.

1Interfacial Structure of Fe-GaAs(001) with annealing and substrate surface morphology

1:27PM J42.00012 Interaction of PH3 with Si(111)-7x7 Surfaces: Adsorption, Desorption and P-segregation. T.-C. SHEN, JEONG-YOUNG JI, Utah State University — The reaction of PH3 with Si(111) surfaces has been studied in the early 1990s by a number of analytical techniques including UPS, AES, EELS and ESD. We are interested in revisiting this system with an emphasis on P-delta layers formation for their potential technological applications. Here we present a STM study of PH3 adsorption on Si(111)-7x7 at 300 K and 900 K. Reacted and unreacted adatom sites after room temperature exposures can be identified by different biases. Similar to the ammonia adsorption the center adatoms are more reactive than corner adatoms. A careful analysis of the surface coverage of PH3, PH2, and H, we conclude that most of PH3 is dissociatively adsorbed on the surface at initial exposure generating H and PH2 adsorption sites followed by molecular adsorption of PH2. More interestingly, a quasi-regular 6√3 surface structure forms by PH3 exposure at 900 K. The dangling bonds of Si(111)-1x1 are completely terminated by a layer of P atoms. No epitaxial Si can be grown on this surface at low temperatures. Annealing the Si covered surface to 900 K recovers the 6√3 structure due to P segregating to the surface. Short heat pulses were used to find that P desorbs at 950 K but 7x7 domain was not observed until 1070 K.

3This work is supported by NSF-NIRT-CCF0404208

1:39PM J42.00013 ABSTRACT HAS BEEN MOVED TO N18.00013 —

Tuesday, March 6, 2007 11:15AM - 2:03PM - Session J43 DMP: Focus Session: Materials for Quantum Information Processing II Colorado Convention Center 506

11:15AM J43.00001 Solid-state materials and devices for single-photon generation and more.

CHARLES SANTORI, Hewlett-Packard — A single-photon device, which ideally emits exactly one photon on demand into a definite quantum state, can be constructed from a single atom or atom-like system excited by optical pulses and coupled to an optical micro-cavity. Solid-state single quantum systems are practical for this application because they do not require complicated trapping setups and can be integrated into monolithic micro-cavity structures. The last several years single-photon generation has been demonstrated in a variety of solid-state systems including nitrogen-vacancy (NV) centers in diamond, epitaxial quantum dots in semiconductors such as InGaAs or AlGaN, and impurities in semiconductors. A variety of microcavity geometries have also been employed to improve photon extraction efficiency and to increase the spontaneous emission rate, including micro-pillars with distributed-Bragg-reflector mirrors, micro-disks and photonic crystal cavities. Results from various systems will be summarized and compared in terms of the suppression of the two-photon emission probability (compared with a Poisson distribution), efficiency, and quantum indistinguishability of the generated photon wave packets. A device that efficiently produces single photons with high spectral purity can also be used in other ways. For example, two photons incident onto such a device should in theory exhibit a strong optical nonlinearity. In addition, if the device uses a three-level Lambda-type system in which two lower long-lived levels are coupled by optical transitions to a common excited state, the possibility exists for efficient matter-photon quantum state inter-conversion, an important ingredient for quantum networks and other applications. It has recently been demonstrated that two solid-state systems, charged quantum dots and nitrogen-vacancy centers in diamond, have the required level structure for this scheme. Recent results demonstrating coherent population trapping in single NV centers will be described which are promising in terms of optical manipulation of single spins and eventually spin-photon inter-conversion.

11:51AM J43.00002 Dynamical nuclear spin polarization and the Zamboni effect in gated double quantum dots. GUY RAMON, XUEDONG HU, Department of Physics, University of Buffalo, SUNY — The hyperfine interaction between electron spins confined in semiconductor quantum dots and the surrounding nuclear spins is one of the main sources for electron spin decoherence in low temperature GaAs quantum dots. We have investigated theoretically the dynamics of a system of two electrons and nuclear spin baths subjected to the hyperfine interaction in a gated double dot system. It is shown that the hyperfine interaction can mediate a dynamical nuclear polarization by utilizing the degeneracy point between the two-electron singlet and polarized triplet states. Most importantly, we demonstrate that a small polarization (0.3%) is sufficient to enhance the singlet decay time by two orders of magnitude, in contrast with the single dot case, where nearly complete nuclear polarization is required to improve spin coherence time significantly. This enhancement is attributed to an equilibration process between the nuclear reservoirs in the two dots, mediated by the hyperfine interaction, an effect we have dubbed as the nuclear Zamboni effect. We explore other strategies to facilitate this effect and show that while equilibration of the two nuclear configurations is obtained, the singlet decay times are only modestly enhanced due to broadening of the nuclear spin distribution.

3Supported by NSA/LPS and ARO

12:03PM J43.00003 Dephasing of exchange coupled spin qubits by electron-phonon coupling. XUEDONG HU, University at Buffalo, SUNY — Exchange coupled spin qubits in semiconductor nanostructures can be dephased by charge fluctuations in the semiconductor environment because of the fundamental Coulombic nature of the Heisenberg coupling. Even when charge fluctuations are suppressed through material improvement, such orbital-degree-of-freedom related fluctuations can still come from electron-phonon interaction in the semiconductor. Here we explore pure dephasing between the two-electron singlet and triplet states for two exchange-coupled spin qubits in a double quantum dot.

4We acknowledge financial support by NSA, LPS, ARO, and NSF
12:15PM J43.00004 Two- and three- energy level mixing effects in vertically coupled quantum dots. CHRIS PAYETTE, DAVID AUSTING, National Research Council of Canada and McGill University, GUOLIN YU, JAMES GUPTA, National Research Council of Canada, SELVA NAIR, University of Toronto, NATIONAL RESEARCH COUNCIL OF CANADA AND MCGILL UNIVERSITY TEAM, NATIONAL RESEARCH COUNCIL OF CANADA TEAM, UNIVERSITY OF TORONTO TEAM — We investigate high bias single electron resonant tunneling through sub-micron gated AlGaAs/InGaAs/AlGaAs/InGaAs/AlGaAs triple barrier structures for which the tunnel coupling energy between the two quantum dots is very weak (less than 0.1meV). The two quantum dot “disks” in the vertical diatomic artificial molecule located in the circular device mesa can be almost circular or elliptically deformed. In a device where the constituent dots are elliptically deformed, the single particle states of each dot evolve almost ideally with magnetic field, except at several of the two- and three- energy level crossings. At these crossing points, we see pronounced two level anti-crossing behavior, with levels split by hundreds of micro-eV, and intriguing level crossing phenomena, like mixing of three resonances leading to resonance suppression. We analyze the observed quantum level mixing effects using a simple three level mixing model.

12:27PM J43.00005 Magnetic field induced resonance and hysteresis effects in the current flowing through coupled vertical quantum dots at high source-drain bias. DAVID AUSTING, CHRIS PAYETTE, National Research Council of Canada and McGill University, GUOLIN YU, JAMES GUPTA, National Research Council of Canada, NATIONAL RESEARCH COUNCIL OF CANADA AND MCGILL UNIVERSITY TEAM, NATIONAL RESEARCH COUNCIL OF CANADA TEAM — We report on the basic properties, including the temperature, range of magnetic field, sweep rate and voltage dependence, of recently observed magnetic field induced resonance and hysteresis effects, which appear through two weakly coupled quantum dots at high source-drain bias. Similar looking effects, attributed to electron spin-nuclear spin (hyperfine) coupling, have been seen in the low bias two- electron spin-blockade regime (K. Ono and S. Tarucha Phys. Rev. Lett. 2004), when the magnetic field is applied perpendicular to the flowing current, but the regime we study here is at much higher bias (up to a few 10’s of mV) and for a magnetic field (0-6T) applied parallel to the current. “Slow” current oscillations/fluctuations are also observed on the timescale of seconds to tens of seconds for certain conditions. Can nuclear spin related effects occur outside the N=2 spin-blockade region?

12:39PM J43.00006 Three-electron bonding and entanglement in single and molecular quantum dots1, YUESONG LI, CONSTANTINE YANNOLEAS, UZI LANDMAN, School of Physics, Georgia Institute of Technology — The study of three-electron quantum dots (QDs) is interesting in several ways. First, it was demonstrated recently that detailed ground-state and excited spectra of few-electron elliptic QDs can be measured as a function of the externally applied magnetic field. Second, three-qubit electron spin devices are expected to exhibit enhanced efficiency for quantum computing purposes compared to single-qubit and two-qubit gates. We carry out exact diagonalization (EXD) studies for a three-electron single QD and for a wide range of anisotropies. We analyze the properties of the EXD many-body wave functions with respect to electron localization in a linear geometry, as well as to generation of model quantum entangled states that are often employed in the theory of quantum computing. We further examine three-electron bonding and entanglement in the case of a double quantum dot.

1Supported by the U.S. D.O.E. (FG05-86ER-45234).

12:51PM J43.00007 Long range spin qubit interaction mediated by microcavity polaritons, CARLO PIERMAROCCHI, GUILLERMO F. QUINTEIRO, Michigan State University, East Lansing, MI 48824, JOAQUIN FERNANDEZ-ROSSIER, University of Alicante, Alicante, 03690 Spain — Planar microcavities are semiconductor devices that confine the electromagnetic field by means of two parallel semiconductor mirrors. When a quantum well (QW) is placed inside a planar microcavity, the excitons in the QW couple to confined electromagnetic modes. In the strong-coupling regime, excitons and cavity photons give rise to new states, cavity polaritons, which appear in two branches separated by a vacuum Rabi splitting. We study theoretically the dynamics of localized spins in the QW interacting with cavity polaritons. Our calculations consider localized electron spins of shallow neutral donors in GaAs (e.g., Si), but the theory is valid for other impurities and host semiconductors, as well as to charged quantum dots. In the strong-coupling regime, the vacuum Rabi splitting introduces anisotropies in the spin coupling. Moreover, due to their photon-like mass, polaritons provide an extremely long spin coupling range. In this work, we present a full analysis of the spin dynamics and compute the coupling flow of the different channels of the system, which is expected to be much longer, a repulsing technique is required. For Hahn echo measurements of T2, a 0-24ns, diffraction-compensating free space THz delay line has been constructed.

1Supported by NSF-NIRT grant CCF 0507295

1:03PM J43.00008 Optically detected quantum dynamics of hydrogenic donor qubits1, DAN ALLEN, SANGWOO KIM, MARK SHERWIN, Department of Physics, UCSB — Orbital states of electrons bound to shallow donors in GaAs provide many of the advantages of trapped atoms for quantum information studies, including optical readout and long lived excited levels. Shallow donors (e.g. S, Si) have a scaled hydrodynamic potential with a bound electron 1S-2P transition at 1 THz (4 meV). In a 5 T magnetic field the 1S state and lowest 2P state (2P−) serve as qubit levels. A cycling transition exists for detecting neutral donors in the ground state via the donor bound exciton resonance; excited bound states are dark. Using this optical quantum nondemolition measurement, the relaxation (T1) of donors after THz excitation of the 1S-2P transition is observed to be > 1µs. High resolution spectroscopy infers that dephasing (T2) of an ensemble of neutral donors is limited by inhomogeneous broadening to 50 ps. In order to measure the decoherence time (T2) which is expected to be much longer, a repulsing technique is required. For Hahn echo measurements of T2 a 0-24ns, diffraction-compensating free space THz delay line has been constructed.

1Supported by NSF-NIRT grant CCF 0507295

1:15PM J43.00009 Characterization of (In,Ga)As Quantum Posts for Terahertz Quantum Information Processing, C. M. MORRIS, D. G. ALLEN, UCSB Physics Dept., J. HE, UCSB Electrical and Computer Engineering Dept., C. PRYOR, University of Iowa Dept. of Physics and Astronomy, P. M. PETROFF, UCSB Electrical and Computer Engineering Dept., M. S. SHERWIN, UCSB Physics Dept. — Quantum posts (QPs) are a new kind of self-assembled semiconductor nanostructure which may be suitable for quantum information processing using terahertz frequencies. A QP is a roughly cylindrical In-rich region embedded in a GaAs matrix whose height can be controlled with monolayer resolution. For a single electron trapped in a 40 nm high QP, the orbital transition between the ground and first excited state is predicted to occur near 1 THz. Since this is well below the optical phonon frequency (9 THz), decoherence is expected to arise primarily from very weak interactions with acoustic phonons. QPs grown in the insulating region of a metal-insulator-semiconductor structure allow voltage-controlled charging, which is measured by capacitance-voltage spectroscopy. Terahertz absorption spectra are also measured by Fourier-transform infrared spectroscopy. 1 M. S. Sherwin, A. Imamoglu and C. Monroy, PRA 60, 3508 (1999) Work supported by the NSF NIRT grant No. CCF 0507295
1:27PM J43.00010 Enhancement of electron spin coherence by optical preparation of nuclear spins. — DIMITRIE STEPANENKO, GUGDO BURKARD, University of Basel, GEZA GIEDKE, Max Planck Institute for Quantum Optics, Garching, ATAC.

IMAGOGLI, ETH Zurich — We study a large ensemble of nuclear spins interacting with a single electron spin in a quantum dot under optical excitation and photon detection. When a pair of applied laser fields satisfy two-photon resonances between the two ground electronic spin states, detection of light scattering from the intermediate exciton state acts as a weak quantum measurement of the effective magnetic (Overhauser) field due to the nuclear spins. If the spin were driven into a coherent population trapping state where no light scattering takes place, then the nuclear state would be projected into an eigenstate of the Overhauser field operator and electron decoherence due to nuclear spins would be suppressed: we show that this limit can be approached by adapting the laser frequencies when a photon is detected. We use a Lindblad equation to describe the time evolution of the driven system under photon emission and detection. Numerically, we find an increase of the electron coherence time from 5 ns to 500 ns after a preparation time of 10 microseconds.

1:39PM J43.00011 Exchange energy in vertically coupled double quantum dots. — TETSUO KODERA, University of Tokyo, JSPS, YOUSUKE KITAMURA, University of Tokyo, KEIJI NO, Riken, SHINICHI AMADA, IROC, YASUHIO TUKURA, IROC, NTT-BRL, SEIGO TARUCHA, University of Tokyo, IROC, UNIVERSITY OF TOKYO TEAM, JSPS TEAM, RIKEN TEAM, IROC TEAM, NTT-BRL TEAM — The exchange separation between spin singlet and triplet states was studied for vertically coupled double quantum dots in the Pauli spin blockade regime with the inter-dot level detuning as a parameter. Pauli blockade is established by the formation of an excited but long-lived triplet state in the double dot, and is lifted by a spin flip transition to the singlet state, generating a leakage current. The leakage current shows a step when the Zeeman energy equals the exchange energy thus turning on the flip-flip interaction with the nuclei. The threshold magnetic field increases on approaching the anti-crossing of the two triplets reflecting the increased exchange energy. We present a quantitative comparison of the exchange energy derived experimentally with exact theory.

1:51PM J43.00012 Electronic structure, entanglement and double occupancy in asymmetric dot molecule quantum gate. — LINXIN HE, Key Laboratory of Quantum Information, USTC, Hefei, Anhui, 230026, P.R. China, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — First, we describe the energy levels, degree of entanglement and double occupancy in fully symmetric (homopolar) quantum dot molecules (QDM) made of InGaAs dots in a GaAs barrier containing ~ 3 x10^9 atoms. We describe the single-particle part by atomistic pseudopotential theory including strain and alloy effects, and the many body part via configuration interaction. Second, we note that in a realistic vertically coupled QDM the two dots often have different geometries, sizes, alloy compositions, (heteropolar QDM) and therefore, deviates from ideal homopolar QDM model used previously. We show that the electronic properties of such heteropolar QDMs are greatly modified by the asymmetry of the QDMs, showing larger two-electron double occupation rate, lower electron entanglement, and therefore reduced quantum gate quality. By symmetrizing the QDM via application of electric field, one can overcome these difficulties.

1 Supported by Chinese NSF Grant No. 60121503 and US.

---

Tuesday, March 6, 2007 11:15AM - 2:03PM — Session J44 DMP: Focus Session: Optical Properties of Nanocrystals Colorado Convention Center 507

11:15AM J44.00001 Polarization-resolved fine structure and magneto-optics of single CdSe nanocrystal quantum dots. — HAN HTOON, Los Alamos National Laboratory — Low-temperature photoluminescence (PL) microscopy of single colloidal quantum dots has proven a very effective tool for probing the emission properties of the band-edge excitons in isolated CdSe nanocrystals (NCs). Past studies employing high spectral resolution have resolved the narrow ‘atomic-like’ emission lines from single NCs, while separately, polarization-resolved measurements have shown that the |1+1> and |1−1> bright exciton states are nominally degenerate with transition dipoles oriented isotropically in the plane normal to the crystallographic c-axis of the NC. To date, however, these two powerful techniques have not been simultaneously employed. To this end we constructed a low-magnification (4 K) microscope to measure both polarization- and spatially-resolved PL of individual nanocrystals. Both orthogonal polarizations (horizontal/vertical linear or right/left circular) are simultaneously recorded to minimize the effects of spectral diffusion and blinking. The data clearly show [1] that many NCs possess a clear bright exciton “fine structure” consisting of two linearly- (and orthogonally-) polarized peaks split in energy by ∆ ≈ 1–2 meV. This splitting is attributed to a breaking of the nanocrystal’s cylindrical symmetry, leading to an anisotropic electron-hole exchange that mixes the |±1> bright excitons. Inferred orientation of the NCs will be discussed. Finally, we study the interplay between the anisotropic exchange and magnetic Zeeman energy in single NCs by incorporating a 5 T magnet into the microscope. With increasing magnetic field, the fine structure states become elliptically polarized and eventually approach pure circular polarization in the limit where the Zeeman energy 1/2gµBB > ∆. We extract the exciton g-factor of individual NCs from the variation of the observed energy splitting with field in this regime.


2 This work is supported by the Los Alamos LDRD program.

11:51AM J44.00002 State-to-state femtosecond relaxation dynamics of excitons in semiconductor quantum dots. — PATANJALI KAMBHAMPATI, SAMUEL SEWALL, RYAN COONEY, KEVIN ANDERSON, EVA DIAS, McGill University — Size dependent exciton relaxation dynamics are measured in colloidal CdSe quantum dots using exciton selective femtosecond spectroscopy. Preparation of the initial exciton state allows evaluation of state-to-state exciton dynamics. These methods reveal the electron and hole relaxation dynamics from a specified initial state to a specified final state, with a precision of 10 femtoseconds. These state selective, size dependent experiments confirm previously observed confinement induced femtosecond Auger channels for electrons with increased precision. This increased precision allows for unambiguous, quantitative evaluation of size dependent transition matrix elements. These experiments furthermore show that the hole relaxation rate increases for smaller quantum dots, contradicting expected relaxation mechanisms for holes. We propose a new confinement enhanced non-adiabatic pathway for hole relaxation in colloidal quantum dots, overcoming the predicted phonon bottleneck for holes. Finally, these experiments show exciton state specific biexcitonic interactions.

12:03PM J44.00003 Size Dependence of Fluorescence Blinking Statistics from CdSe Nanorods. — SIYING WANG, CLAUDIA QUERNER, University of Pennsylvania, THOMAS EMMONS, Swarthmore College, MARIJA DRNDIC, University of Pennsylvania, CATHY CROUCH, Swarthmore College — We report fluorescence blinking statistics measured from single CdSe nanorods (NRs) of seven different sizes with aspect ratios ranging from 3 to 11. The off-times follow a power-law probability distribution; on-times follow a truncated power law distribution, P(on) ~ τon/τc. At fixed excitation intensity, the truncation rate 1/τon increases with increasing aspect ratio. For a particular sample, 1/τon increases gradually with increasing excitation intensity. Examining 1/τon vs. single-particle photon absorption rate for all samples indicates that the shape dependence of the absorption cross-section does not fully account for the observed variation in crossover time τc. Surprisingly, we observe no significant difference between core and core/shell nanorods or core rods with different surface ligands. Our results suggest that NR internal structural defects or degree of quantum confinement may contribute to the shape dependence of the crossover time.

3 This work was funded by ONR, NSF, and HHMI.
12:15PM J44.00004 Size and shape dependence of CdSe nanocrystal band-edge exciton fine structure1, QINGZHONG ZHAO, KWSEON KIM, PETER A. GRAF, WESLEY B. JONES, ALBERTO FRANCESCHETTI, National Renewable Energy Laboratory, LIN-WANG WANG, Lawrence Berkeley National Laboratory — Advances in growth methods of nanocrystals led to controlled synthesis over size and shape, influencing their optical properties. Ground exciton states of CdSe nanocrystals are shown to be sensitive to their geometries. We investigate the exciton fine structure of CdSe nanocrystals using empirical pseudopotential and configuration interaction methods1,2. Systematic studies of the size and shape dependency are performed on the band edge states of CdSe spherical quantum dots, elongated nanorods, flattened nanodisks, nanowires and quantum wells. Large scale electronic band structures for diameters from 1.8 nm and lengths from 2 to 11 nm were calculated. We explore size and shape dependence of exciton fine structure over the diameter-length space and explain it by the interplay of quantum confinement, crystal field splitting, and exchange interaction. We find the experimentally observed dark-bright exciton crossing1 and discuss its size shape dependency. [1] L. W. Wang and A. Zunger, Phys. Rev. B 51, 17398 (1995). [2] A. Franceschetti, et al., Phys. Rev. B 60, 1819 (1999). [3] N. Le Thomas, et al., Phys. Rev. Lett. 94, 016803 (2005). *This work was supported by US DOE-SC-BES and ASCR TMSN Initiative.

12:27PM J44.00005 Ab initio Theory of Semiconductor Nanocrystals1, LIN-WANG WANG, Lawrence Berkeley National Laboratory — With blooming experimental synthesis of various nanosstructures out of many semiconductor materials, there is an urgent need to calculate the electronic structures and optical properties of these nanosystems based on reliable ab initio methods. Unfortunately, due to the O(N^3) scaling of the conventional ab initio calculation methods based on the density functional theory (DFT), and the >1000 atom sizes of the most experimental nanosystems, the direct applications of these conventional ab initio methods are often difficult. Here we will present the calculated results using our O(N) scaling charge patching method (CPM) [1] to nanosystems up to 10,000 atoms. The CPM yields the charge density of a nanosystem by patching the charge motifs generated from small prototype systems. The CPM electron-hole energy eigners differ from the directly calculated results by only ~10-20 meV. We will present the optical band gaps of quantum dots and wires, quantum rods, quantum dot quantum well, and quantum dots doped with impurities. Besides good agreements with experimental measurements, we will demonstrate why it is important to perform ab initio calculations, in contrast with the continuum model k.p calculations. We will show the effects of surface polarization potentials and the internal electric fields. Finally, a linear scaling 3 dimensional fragment local spin density functional theory (LS3DF) method will be discussed. The LS3DF method can be used to calculate the total energy and atomic forces of a large nanosystem, with the results practically the same as the direct DFT method. Our work demonstrates that, with the help of supercomputers, it is now feasible to calculate the electronic structures and optical properties of >10,000 atom nanocrystals with ab initio accuracy. [1] L.W. Wang, Phys. Rev. Lett. 88, 256402 (2002).

1This work was supported by U.S. Department of Energy, BES/SC, under Contract No. DE-AC02-05CH11231 and used the resources of the National Energy Research Scientific Computing Center.

1:03PM J44.00006 Size-dependent optical spectrum of CdSe nanocrystals, W. JASKOLSKI, Instytut Fizyki UMK, Torun, Poland, G.W. BRYANT, J.G. DIAZ, NIST, Gaithersburg, MD 20899-8423 — An empirical sp^3d^5 tight-binding model has been employed to describe the optical properties of CdSe nanocrystals on a wide range of sizes. The sp^3d^5 model explains successfully the single-particle electron levels and excitonic effects including the evolution of both the emission and absorption peaks with confinement. We provide an interpretation of the band-edge fine structure in agreement with both the one- and two-photon spectroscopies and the PLE resonant and non-resonant Stokes shifts. Previous effective mass, pseudopotential and sp^3^a tight-binding models were unable to explain such experiments. The wurtzite lattice structure splits the lowest S- and P- hole states into two doublets that overlap, in accordance to the indistinguishability observed between the one-photon and two-photon spectroscopies. A correct description of the spin-orbit coupling allows the non-resonant Stokes shift to be reproduced. Finally, for dot radius below 2.3 nm, an optically passive P- level becomes the ground hole state giving rise to the large resonant Stokes shift observed experimentally.

1:15PM J44.00007 Carrier Multiplication in PbSe Quantum Dots, ALBERTO FRANCESCHETTI, JOONHEE AN, ALEX ZUNGER, National Renewable Energy Laboratory — The efficiency of conventional solar cells is limited, because the energy of absorbed photons in excess of the band gap is converted to heat, instead of producing electron-hole pairs. Recently, efficient carrier multiplication has been observed in siconductor quantum dots. In this process, a single, high-energy photon generates two or more electron-hole pairs, thus potentially increasing the efficiency of solar cells. Rather exotic mechanisms have been proposed to explain carrier multiplication in PbSe quantum dots. Using atomistic semi-empirical pseudopotential calculations, we show that the more conventional impact ionization mechanism - whereby a photogenerated electron-hole pair decays into a biexciton in a process driven by Coulomb interactions between the carriers - can explain both the rate (< 1 ps) and the energy threshold (~ 2.2 times the band gap) of carrier multiplication in PbSe quantum dots [1,2], without the need to invoke alternative mechanisms. The reason is that the density of biexciton states increases very rapidly with energy, thus making the rate of impact ionization faster than the rate of competing decay channels. [1] A. Franceschetti, J.M. An and A. Zunger, Nano Letters, 6, 2191 (2006). [2] J.M. An, A. Franceschetti and A. Zunger, Nano Letters, n061684x (2006).

1:27PM J44.00008 Optical Properties of PbSe Nanocrystal Quantum Dots Under Pressure3, KIRILL K. ZHURAVEV, JEFFREY M. PIETRYGA, ROBERT K. SANDER, RICHARD D. SCHALLER, Los Alamos National Laboratory — The optical properties of PbSe nanocrystal quantum dots (NQDs) were studied as a function of applied hydrostatic pressure over the range from ambient to 4 GPa. PbSe NQDs exhibit an energy gap that is dominated by quantum confinement energy. Despite such strong confinement, we find that the energy gaps of 3, 5, and 7 nm PbSe NQDs change monotonically with pressure with a dependence that is almost entirely determined by the deformation potential. The sizable dependence of the NQD energy gap with pressure invites applications in the areas of high speed pressure sensing and tunable IR lasers. We will also present x-ray diffraction data, including the data indicating new phase transition not observed earlier.

3This work was supported by the US Department of Energy under contract W-7405-ENG-36 and the Intelligence Technology Innovation Center. JMP was supported by an Intelligence Community Research Fellowship. RDS was supported by a Frederick Reines Fellowship.

1:39PM J44.00009 Theory of InP nanocrystals under pressure, J.G. DIAZ, G.W. BRYANT, W. JASKOLSKI, National Institute of Standards and Technology, Gaithersburg, MD 20899-8423 — An empirical tight-binding theory which includes the effects of the relaxation of the lattice is employed to investigate the role of an external hydrostatic pressure on the opto-electronic properties of InP nanocrystals. For the bulk, our model describes accurately the evolution of the lowest conduction band-edges with pressure and predicts the \Gamma_{1c}-X_{1c} crossover at the same lattice contraction as measured in the experiment. For small InP nanocrystals, the bandgap dependence on pressure predicted with this model is, for the first time, in agreement with the experimental results. Previous atomistic models, which assumed a bulk-like arrangement for the atoms in the nanocrystal under pressure, led to negligible mixing of the \Gamma_{1c} and \Gamma_{1s} minima and did not account for the increasing localized character of the electron and hole states as a function of pressure. The lattice-relaxed tight-binding model suggests a mechanism for the experimental red-shift different from the \Gamma_{1c}-X_{1c} crossover predicted by bond-distance scaling models. In the lattice-relaxed model, the experimental red-shift is explained as a transition from bound states localized inside the dot to surface-like states in the dot exterior. The evolution of the near-band-edge optical spectra as a function of pressure has been analyzed for different nanocrystal sizes, geometries and degrees of surface passivation with both the bond-length scaling and lattice-relaxed tight-binding approaches.
Enabling Superconductivity — The DOE Basic Energy Sciences Workshop on Basic Research Needs for Superconductivity identified grand challenges and research priorities for discovery and use inspired basic research to transform the US power grid to meet the needs of the 21\textsuperscript{st} century. Vortex matter research is central to this endeavor and helps support both fundamental and applied research. The science of vortex matter embodies the fundamental mysteries of vortex-vortex interactions in an inhomogeneous and anisotropic matrix. Understanding the complex phase diagrams and the dynamic responses that result from these competing effects is an outstanding challenge. Simultaneously, the prospect of controlling these interactions opens new horizons for basic research such as the development of a microscopic theory for vortex dynamics, exploration of vortex nucleation at magnetic and superconducting interfaces and designs for pinning a vortex liquid at high temperatures. This presentation will highlight ways in which nanotechnology based methodologies, dynamic vortex creep phenomena and powerful computer simulations play a role in enhancing our understanding of next-generation and new classes of superconductors.

Supported by NSF Grant DMR-0421810.

5:44PM L1.00005 Transforming the Grid with Superconductivity, ALEXIS MALOZEMOFF, American Superconductor Corporation — The electric power grid in the United States faces critical challenges: overloading caused by years of limited investment and steady load growth, bottlenecks in power corridors into urban centers, voltage instability leading to brownouts and blackouts, growing fault currents in large urban and suburban areas, as well as the need for increased efficiency. Power equipment based on high temperature superconductors (HTS) offers solutions to these challenges: high capacity, non-interfering HTS cables addressing power bottlenecks, HTS fault current limiters controlling fault currents, HTS synchronous condensers and novel controllability features of HTS cables which address stability issues, HTS transformers and generators with increased efficiency. A variety of commercial-level demonstrations make the impact of HTS power equipment imminent. The fluorescence of the QDs was found to be retained within the cylindrical nanopores of PAMs.
2:30PM L11.00001 Flow diagram of the metal-insulator transition in two dimensions1 , SERGEY
KRAVCHENKO, Northeastern University, SVETLANA ANISSIMOVA, Boston University, ALEXANDER PUNNOOSE, CCNY, ALEXANDER FINKEL’STEIN,
Weizmann Institute, TEUN KLAPWIJK, TU Delft — Recently, a two-parameter scaling theory comprehensively describing the metal-insulator transition in 2D
was developed by two of us [1]. Here, we report experimental verification of the basis of this theory. We demonstrate, for the first time, that as a result of the
interplay between the electron-electron interactions and disorder, both the resistance and the interactions become scale (temperature) dependent. We show that
not only the resistance but also the interaction amplitude exhibits a fan-like spread as the MIT is crossed. We use these data to construct a resistance-interaction
flow diagram of the MIT that clearly reveals a quantum critical point, as predicted in Ref.[1]. The metallic side of this diagram is accurately described by the
theory without any fitting parameters. In particular, the temperature dependence of the resistance, which is non-monotonic, passes through a maximum when
the interaction amplitude reaches a certain value γ2 ≈ 0.45 that is in remarkable agreement with the calculated one.
1 Supported

by NSF, ACS, and Minerva Foundation

2:42PM L11.00002 Quantum Coulomb glasses and electron assisted hopping , MARKUS MULLER, Harvard
University, LEV IOFFE, Rutgers University — In Anderson insulators where the single particle localization length is much larger than the mean distance between
electrons, Coulomb interactions drive the electrons into a strongly correlated quantum glass phase. In the limit of large localization length, the resulting quantum
Coulomb glass can be studied analytically. The theory predicts many almost degenerate quantum states with a spectrum of gapless collective excitations in
each of them. The latter can acts as a bath with which individual electrons can exchange energy. This is a crucial ingredient for activated transport, the
collective modes of the quantum glass providing a natural mechanism for electron-assisted hopping conductance. In particular, for 2D systems we predict a
weakly temperature dependent pre-exponential factor of order e2 /h for variable range hopping, as has been reported in many recent experiments.
2:54PM L11.00003 Multifractality and Conformal Invariance at 2D Metal-Insulator Transition
in the Spin-Orbit Symmetry Class , HIDEAKI OBUSE, RIKEN, Japan, ARVIND SUBRAMANIAM, University of Chicago, AKIRA FURUSAKI, RIKEN, Japan, ILYA GRUZBERG, University of Chicago, ANDREAS LUDWIG, University of California, Santa Barbara — We study the multifractality
of critical wave functions at boundaries and corners at the Anderson metal-insulator transition for noninteracting electrons in the two-dimensional (2D) spin-orbit
(symplectic) universality class. We find that the multifractal exponents near a boundary are different from those in the bulk. The exponents at a corner are
found to be directly related to those at a straight boundary through a relation arising from conformal invariance. This provides direct numerical evidence for
conformal invariance at the 2D spin-orbit metal-insulator transition. We also show that the presence of boundaries modifies the multifractality of the whole
sample even in the thermodynamic limit.

3:06PM L11.00004 Localization of interacting fermions at high temperature , VADIM OGANESYAN, Yale
University, DAVID HUSE, Princeton University — We suggest that if a localized phase at nonzero temperature T > 0 exists for strongly disordered and weakly
interacting electrons, as recently argued, it will also occur when both disorder and interactions are strong and T is very high. We show that in this high-T
regime the localization transition may be studied numerically through exact diagonalization of small systems. We obtain spectra for one-dimensional lattice
models of interacting spinless fermions in a random potential. As expected, the spectral statistics of finite-size samples cross over from those of orthogonal
random matrices in the diffusive regime at weak random potential to Poisson statistics in the localized regime at strong randomness. However, these data show
deviations from simple one-parameter finite-size scaling: the apparent mobility edge “drifts” as the system’s size is increased. Based on spectral statistics alone,
we have thus been unable to make a strong numerical case for the presence of a many-body localized phase at nonzero T .
3:18PM L11.00005 Out-of-Equilibrium Dynamics of a Strongly Correlated Electron System in
Two Dimensions1 , DRAGANA POPOVIĆ, National High Magnetic Field Laboratory (NHMFL) and Department of Physics, Florida State University
(FSU), JAN JAROSZYŃSKI, NHMFL, FSU — Slow, nonexponential relaxations of conductivity σ(t) have been studied in a strongly disordered two-dimensional
electron system (2DES) in Si MOSFETs in the vicinity of the metal-insulator transition (MIT). The 2DES is excited far from equilibrium by a rapid change of
carrier density ns at low temperatures T . The dramatic and precise dependence of σ(t) on ns and T shows that (a) the equilibration time diverges exponentially
as T → 0, suggesting a glass transition at Tg = 0, and (b) the Coulomb interactions between 2D electrons play a dominant role in the observed out-of-equilibrium
dynamics [1]. The scaling of σ(t, T ) is also consistent with Tg = 0. These results support conclusions based on earlier noise measurements [2] that, in a 2DES
in Si, the glass transition occurs in the metallic phase as a precursor to the MIT.
1 Supported

by NSF grant DMR-0403491 and NHMFL through NSF Cooperative Agreement DMR-0084173.

3:30PM L11.00006 Electric field gating near the metal-insulator transition using ionic liquid
dielectrics1 , ARTHUR HEBARD, RAJIV MISRA, MITCHELL MCCARTHY, University of Florida — Ionic liquids (ILs) are highly polar low-meltingtemperature binary salts typically comprising nitrogen-containing organic cations and inorganic anions. Since there is no solvent, ILs are distinctly different from
aqueous, organic, gel or polymer electrolytes. Using either coplanar or overlay gate configurations in which the IL is the gate dielectric, we demonstrate room
temperature field-induced resistance changes on the order of a factor of 104 for thin conducting InOx films. There is a large asymmetry manifested by the
significantly larger changes in impedance for negative gate voltage Vg (electron depletion) compared to positive Vg (electron enhancement). The pronounced
frequency dependence over the range 10−2 –106 Hz, due to the low ionic mobilities in the dielectric fluid, is modeled well by a simple RC circuit from which an
effective areal gate capacitance can be derived. The induced surface charge densities and field-effect mobilities noticeably exceed those that can be achieved
on similar films using AlOx dielectrics. In addition, the charge state can be frozen in by reducing the temperature below the glass transition (∼250K) of the IL,
thus providing an opportunity for electric field tuning of metal-insulator transitions in a variety of novel thin-film systems.
1 Work

supported by the NSF under Grant #0404962


3:42PM L11.00007 Phase diagram of amorphous Ta thin films in B-T-disorder space, YIZE LI, YONGGUANG QIN, CARLOS VICENTE, JONGSOO YOON, University of Virginia — We have studied the effect of temperature (T) and perpendicular magnetic fields (B) on the transport properties in amorphous Ta thin films. In the zero T limit, the films exhibit superconducting, metallic, and insulating phases with increasing B. Each phase can be identified by distinct nonlinear current-voltage (I-V) characteristics: the I-V curves in the superconducting phase are characterized by a hysteresis, in the metallic phase the differential resistance (dV/dI) increases with increasing I, while in the insulating phase dV/dI decreases with increasing I [1]. As demonstrated for the superconducting and metallic phase, these nonlinear transports arise from a non-thermal origin [2]. In order to understand the effect of B, T, and disorder on the electronic states and the nature of the resulting ground states, we construct a B-T-disorder space “phase diagram”. Disorder is controlled by film thickness. The resulting phase diagram shows that the superconducting phase is completely surrounded by the metallic phase, in the zero temperature limit (B-disorder plane) a B-induced direct superconductor-insulator transition is not allowed, while a superconductor-metal-insulator or metal-insulator transition are possible depending on the degree of disorder in our 2D system. [1] Y. Qin et al., Phys. Rev. B 73, 100505(R) (2006). [2] Y. Sato et al., Phys. Rev. Lett. 97, 057005 (2006).

3:54PM L11.00008 Local structural aspects of the metal-insulator transition in CuIr2S4 from total scattering x-ray study1, EMIL BOZIN, HYUN JONG KIM, AHMAD MASADEH, SIMON BILLINGE, Michigan State University, JOHN MITCHELL, Argonne National Laboratory — A thiopenal CuIr2S4 exhibits a metal-insulator (MI) transition at T=230 K, with simultaneous spin-dimerization and charge-ordering [1]. The transition can also be driven by extended exposure to the x-rays at low T [2]. Total x-ray scattering study of CuIr2S4 was carried out using 100 keV synchrotron beam and rapid acquisition pair distribution function (RAPDF) approach [3]. The RAPDF results indicate consistency of the local and the average structure at high T. At 100 K a long-x-ray exposure melts the long-range order (LRO) of the dimerization pattern, without affecting the local structure, in agreement with diffuse scattering result [2]. The dependence of the LRO related superlattice peak intensity on the exposure time reveals that the melting occurs within approximately 15 seconds of exposure under experimental conditions used. At 100 K the LRO is recovered without temperature increase quickly after the cessation of the beam exposure. [1] P.G. Radaelli et al., Nature 416, 155 (2002). [2] H. Ishibashi et al., Phys. Rev. B 66, 144424 (2002). [3] P.J. Chupas et al., J. Appl. Cryst. 36, 1342 (2003).

4:06PM L11.00009 First-order metal-insulator transition and structural phase transition: analysis of coherent phonons observed by femtosecond pulse laser in VO2, HYUN-TAK KIM, BYUNG-GYU CHAE, BONG-JUN KIM, YONG WOOK LEE, SUN JIN YUN, KWANG-YONG KANG, ETRI in Korea, KANG-JEON HAN, KI-JU LEE, Chugmang U., YONG-SIK LIM, Konkuk U. — It has been well-known that VO2 undergoes both a structural phase transition (SPT) (electron-phonon interaction) from monoclinic (insulator phase) to tetragonal (metal phase) and of a discontinuous first-order metal-insulator transition (MIT) (Jump) (electron-electron interaction) near 68°C. Peierls transition and Mott transition in VO2 remain controversial. We have investigated a relation of the MIT and the SPT in VO2 by observing coherent phonons using a laser with a femtosecond pulse width (10~20 fs). A coherent phonon indicating a metal phase is measured after MIT. This indicates that the SPT does not affect the MIT. This is confirmed by a micro-Raman scattering experiment and XRD. The speed of the first-order MIT is interpreted as about 100 femtosecond. This is different from a well-known analysis in which the SPT and the MIT simultaneously occur. (References on the MIT: New J. Phys. 6 (1994) 52 (http://www.njp.org), Appl. Phys. Lett. 86 (2005) 242101, Physica B 369 (2005) 76; cond-mat/0607577; cond-mat/0608085; cond-mat/0609033)

4:18PM L11.00010 Spin-Valley Phase Diagram of the 2D Metal-Insulator Transition, O. GUNAWAN, T. GOKMEN, K. VAKILI, M. PADMAÑABHAN, E.P. DE POORTERE, M. SHAYEGAN, Princeton University, SHAYEGAN’S GROUP TEAM — It has been recognized that the spin degree of the freedom plays a crucial role in the controversial metal-insulator transition problem in 2D carrier systems. Here, we directly probe the role of another discrete electronic degree of freedom, namely the valley polarization. Using symmetry breaking strain to tune the valley occupation of a 2D electron system an AlAs quantum well, together with an applied in-plane magnetic field to tune the spin polarization, we map out a spin-valley phase diagram for the 2D metal-insulator transition. The insulating phase occurs in the quadrant where the system is both spin- and valley-polarized. This observation establishes the equivalent roles of spin and valley degrees of freedom in the 2D metal-insulator transition.

4:30PM L11.00011 Doping variation of orbitally-induced anisotropy in electronic structure of the perovskite-type vanadium oxides, JUN FUJIOKA, SHIGEKI MIYASAKA, Dept. of Appl. Phys., Univ. of Tokyo, YOSHINORI TOKURA, Dept. of Appl. Phys., Univ. of Tokyo, ERATO-SSS, AIIST–CERC — Recently, the perovskite-type vanadium oxide LaV3O10 has been attracting much attention. In this system, the anisotropic charge dynamics due to the one-dimensional orbital exchange interaction is observed. In addition, the filling control insulator-metal transition (FC-IMT) concomitant with the orbital ordering-disordering transition can be achieved in the hole doped system La1−xSr2+3xV2O4. [1]. In this study, the variation of anisotropic charge dynamics in the course of FC-IMT in the perovskite-type vanadium oxide has been investigated by measurements of optical conductivity spectra with focus on the role of t2g-orbital degree of freedom. The orbitally-induced anisotropic feature of the Mott-gap excitation as well as the doping-induced mid-infrared excitation is suppressed with increasing the hole concentration, and instead the isotropic and incoherent dynamics of the doped hole dominates over the low-energy excitation near and above the MIT point.


4:42PM L11.00012 Screening of disorder by the Hubbard interaction near a metal-insulator transition in two dimensions1, PRABUDDHA CHAKRABORTY, University of California, Davis, PETER DENTENEER, Lorentz Institute, LION, Leiden University, Leiden, The Netherlands, RICHARD SCALETTER, University of California, Davis — We present a determinant quantum Monte Carlo study of the metal-insulator transition in the Hubbard model on a square lattice with random site disorder. We show that beyond a critical value of the Hubbard interaction U, the Anderson insulator can undergo a phase transition to a two-dimensional metal. It is also shown that a further increase of the Hubbard interaction can lead to a decrease in conductivity, in direct analogy with the superfluid to Bose-glass transition in the bosonic Hubbard model. We point out that screening of disorder by the Hubbard interaction is not enough to explain the metal-insulator transition in the two-dimensional disordered Hubbard model.

1Support from National Science Foundation under NSF DMR 0312261 and NSF DMR 0421810.
4:54PM L11.00013 The metal to insulator transition in manganites - evidence for changes in the kinetic energy up to 24 eV, I. MAHNS, A. RUDSCHY, G. NEUBER, M. BASTJAN, S. MUELLER, P. SAICHIU, B. SCHULZ, M. RIEUBHAUSEN, IAP, University of Hamburg, Germany, R. RAUER, Dept. of Applied Physics, Chalmers University of Technology, Goeteborg, Sweden, G. STRYGANYUK, Insti. f. Exp.Physik, University of Hamburg, Germany, K. DOERR, IFW Dresden, Germany, G. A. SAWATZKY, Dept. of Physics & Astronomy, University of British Columbia, Vancouver, Canada — The electronic response of doped manganites at the transition from the paramagnetic insulating to the ferromagnetic metallic state in La$_{1-x}$Ca$_x$MnO$_3$ and La$_{1-x}$Ca$_x$MnO$_2$ was investigated by a combination of dc conductivity, ellipsometry, and VUV-reflectance measurements covering an energy range from 0 to 24 eV. By performing a stabilized Krammer-Kronig transformation, we obtain the optical conductivity as a function of temperature around the metal to insulator transition. Our main findings are that changes in the kinetic energy exceed energies of more than 22 eV. In the spectral range between 0 and 24 eV the spectral weight is conserved within a fraction of 3/1000. The pronounced redistribution of the spectral weight between low and high energies has important ramifications for the construction and down-folding of effective low-energy Hamiltonians. We discuss the importance of local interactions to the electronic bandstructure such as the Coulomb onsite and Jahn-Teller effects.

5:06PM L11.00014 Metal-Insulator Transition and Coulomb Gap: A Real-Space Dynamical Mean-Field Study of the Anderson-Hubbard Model, YUN SONG, W.A. ATKINSON, R. WORTIS, Department of Physics & Astronomy, Trent University, 1600 West Bank Drive, Peterborough, Ontario, Canada K9J 7B8 — The interplay between disorder and electron interactions in the two-dimensional paramagnetic Anderson-Hubbard model is studied by real-space dynamical mean-field theory (DMFT) with a Hubbard-I solver. At half-filling, the Mott gap evolves into a Coulomb-like gap with power law energy dependence $|E - E_F|$, suggesting a Mott insulator to Anderson insulator transition as a function of disorder. Away from half filling for strong interactions and disorder, we find a negative density of states (DOS) anomaly at the Fermi level that is distinct from the Mott gap. Far from half filling, we obtain a positive DOS anomaly at the Fermi level. While this positive anomaly is consistent with paramagnetic mean-field calculations, the negative anomaly near half filling is a feature unique to strong correlation physics.

5:18PM L11.00015 Jastrow theory of the Mott transition in bosonic Hubbard models, MANUELA CAPELLO, Laboratoire de Physique Theorique, Universite de Toulouse, FEDERICO BECCA, MICHELE FABRIZIO, SANDRO SORELLA, International school for advanced studies SISSA (Trieste) — We show that the Mott transition occurring in bosonic Hubbard models can be successfully described by a simple variational wave function that contains all important long-wavelength correlations. Within this approach, a smooth metal-insulator transition is made possible by means of a long-range Jastrow correlation term that binds in real space density fluctuations. We find that the Mott transition has similar properties in two and three dimensions but differs in one dimension. We argue that our description of the Mott transition in terms of a binding-unbinding transition is of general validity and could also be applied to realistic electronic systems.

Tuesday, March 6, 2007 2:30PM - 5:30PM – Session L12 GMAG DMP FIAP: Focus Session: Magnetic Semiconducting Oxides

2:30PM L12.00001 Challenges in the Synthesis of Diluted Magnetic Semiconducting Oxides, THIRUMALAI VENKY VENKATESAN, University of Maryland and Neocera — In the rapidly advancing field of Spintronics, the quest for an above room temperature diluted magnetic semiconductor (DMS) has been thwarted by the lack of a conventional semiconductor with above room temperature ferromagnetism (FM). The recent observation of high temperature FM in numerous oxides has created a flurry of publications with controversial results. I will address the origin of this controversy and trace it to the fact that unlike their predecessors, the manganites, which had significantly large magnetization signals, we are now dealing with samples of weaker magnetization and the measurements are vulnerable to extraneous effects. With the example of Co doped TiO$_2$, I will show that the substitutional incorporation of the magnetic ion in the host lattice is a process dependent phenomenon and Co incorporation and the lattice crystallization have opposing behavior with temperature. The role of TEM-EELS and XAS in distinguishing between intrinsic vs. extrinsic effects will be delineated. There are process regimes in which a homogeneously doped TiO$_2$ DMS system does exist while in the rest of the region one obtains a super paramagnetic system with Co clusters embedded in a TiO$_2$ host. Results from anomalous Hall and field effect studies will be discussed and other magnetically doped oxide host systems will also be covered.

3:06PM L12.00002 Room temperature ferromagnetism in Fe-doped TiO$_2$ films is unrelated to magnetic ordering of iron. M VENKATESAN, CRANN and School of Physics, Trinity College, Dublin 2. Ireland, R.D. GUNNING, J.M.D. COEY, MANSE TEAM — TiO$_2$$_{2-x}$ films doped with $x = 1 - 5$ at.% $^{57}$Fe produced in oxidizing or reducing conditions by pulsed laser deposition on sapphire substrates exhibit ferromagnetic behaviour at room temperature. Conversion electron Mössbauer spectra show that most of the iron in the oxidized film (10$^2$ Pa) is present as paramagnetic Fe$^{3+}$ or Fe$^{4+}$ whereas in the reduced films (10$^{-1}$ Pa) most of the iron is present as well crystallized iron metal. The moment per iron atom for 1% and 5% films significantly exceeds the value of 2.2 $\mu_B$ for iron metal and in the 1% oxidized film it is as much as 6.9 $\mu_B$ per iron atom. Films where the dopant ions are not magnetically ordered possess some of the largest ferromagnetic moments. Saturation moments are in the range 2-20 $10^{-8}$ Am$^2$ or 90-900 $\mu_B$ nm$^{-2}$ of substrate area. The iron in these oxidized films is in Fe$^{3+}$ or Fe$^{4+}$ state, but it is not magnetically ordered and cannot therefore contribute to the observed ferromagnetic moments. The isomer shifts indicate octahedral oxygen co-ordination for both ions. We conclude that Fe-doped TiO$_2$ cannot be regarded as dilute magnetic semiconductor. The magnetism of this, and may be that of many other dilute magnetic oxides might be explained in terms of oxygen-based electronic defects, or orbital currents which do not involve the dopant directly.

3:18PM L12.00003 Room temperature ferromagnetism in Mn and Fe-doped indium-tin oxide films, J.M.D. COEY, CRANN and School of Physics, Trinity College, Dublin 2. Ireland, R.D. GUNNING, M VENKATESAN, MANSE TEAM — Following the reports of high temperature ferromagnetism in n-type Mn-doped Indium tin oxide (ITO) thin films, we have undertaken a systematic investigation of the magnetic and transport properties of ITO thin films doped with all the 3d transition metal ions. ITO films were grown on c-cut sapphire substrate by pulsed laser deposition. The X-ray diffraction patterns reveal that they are oriented mainly in (111) direction of cubic bixbyite structure. Undoped ITO films are diamagnetic. Room temperature ferromagnetism is observed in Fe and Mn-doped thin films of varying concentrations, when deposition temperatures are greater than 600 °C. The largest magnetic moments were found in 2.5% Mn-doped and 7.5% Fe-doped ITO films. The Mn-doped films are anhysteretic, while the Fe-doped films exhibit a hysteresis with a coercivity of 30 mT and a moment which increases with concentration. However, in the Mn-doped samples, we see a higher moment for the lower concentrations. None of the other doped ITO films were found to be magnetic, ruling out the possibility of cluster based magnetism. Conversion electron Mössbauer spectra of the ferromagnetic iron-doped films show the presence of magnetite in quantities sufficient to explain the magnetization. No such secondary phase is found for Mn.
3:30PM L12.00004 Room Temperature Ferromagnetism in Mn-implanted CVD-Grown ZnO Films and Nanostructures1, D. HILL, R. GATEAU, R.A. BARTYNISKI, P. WU, Y. LU, L. WIEILINSKI, V. POLTAVETS, M. GREENBLATT, Rutgers University, D.A. ARENA, Brookhaven National Lab., J. DVORAK, Montana State University, A. MOODENBAUGH, Brookhaven National Lab., S. CALVIN, Sarah Lawrence College — We have characterized the chemical, compositional, and magnetic properties of Mn-ion implanted epitaxial ZnO films and single crystal nanostructures grown by MOCVD as candidate room temperature diluted magnetic semiconductors. X-ray absorption spectroscopy (SXAS) and EXAFS show that the as Mn-implanted films contain isolated Mn3+ ions substitutional for Zn. Upon annealing the distribution of Mn ions changes becomes locally enriched with a substantial fraction of the nearest cation being Mn. SQUID magnetometry shows that as-implanted films are ferromagnetic at 5K with a saturation magnetization of \( \sim 0.2 \mu_B/\text{Mn-ion} \). The annealed films have an Ms that is \( \sim 1 \mu_B/\text{Mn-ion} \) and are ferromagnetic at room temperature. Elemental analysis of the nanorods in the transmission electron microscope shows that the Mn concentration is relatively uniform perpendicular to the axis of the structure, but has a higher concentration near the tip than at the base.

3:42PM L12.00005 A comparative RIXS study on Co2+ systems, DIETER SCHMEISSER, BTU Cottbus, JONATHAN DENLINGER, Advanced Light Source — We use RIXS at the ALS BL8 to investigate systems in which Co is preferentially in the Co2+-state. The systems include Co:ZnO, Co2O3, Co doped in polypyrrole, Co-phthalocyanine films, and CoO. For all these systems we report on the XAS and RIXS data at the Co2p edge. We separate the inelastic Raman losses due to d-d excitations from valence band induced excitations. We identify and quantify the relative contributions of the d7 HS and LS states and d8L charge transfer states.

3:54PM L12.00006 V, Nb and Ta doping of anatase TiO2: a from a dilute magnetic semiconductor to a transparent conducting oxide3, JORGE OSORIO-GUILLÉN, STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — We have investigated by means of first-principle supercell calculations the effects of doping anatase TiO2 by V, Nb and Ta. We find: (i) V doping makes TiO2:V ferromagnetic. A single V impurity has a magnetic moment of 1.0 \( \mu_B/\text{V atom} \) with an electronic configuration \( t_2^2 e_g^4 \). The ferromagnetic interaction between two V impurities is found to extend to more than five neighbors, with calculated ferromagnetic stabilization energy ranging from 124 meV at the first neighbor to 27 meV at the fifth neighbor. (ii) Nb and Ta doping of TiO2 makes the system conductive, but not magnetic. The calculated equilibrium free-electron concentration \( n_s \) at \( T = 1000K \) for Ti-rich--O-poor growth conditions is \( 2.7 \times 10^{21} \) and \( 5.9 \times 10^{21} \) cm\(^{-3} \) for Nb and Ta doping respectively, whereas pure TiO2 is calculated to have a electron density of only \( 1.8 \times 10^{18} \) cm\(^{-3} \) due to intrinsic defects. Thus, Nb and Ta doping of TiO2 enhance dramatically the electron concentration and hence are good transparent conductor oxides.

This work was funded by DARPA under NREL contract No. DE-AC36-99GO10337

4:06PM L12.00007 room temperature ferromagnetism in Zn1-xFe2O3:S. KOLESNIK, B. DABROWSKI, O. CHMAISSEM, Department of Physics, Northern Illinois University, DeKalb, IL, W. L. LIM, Department of Physics, University of Notre Dame, Notre Dame, IN, M. PEKALA, Department of Chemistry, Warsaw University, Warsaw, Poland — Room temperature ferromagnetism in Zn1-xFe2O3 can be obtained by precipitation of ZnFe2O4 impurity phase (with the Curie temperature of 440 K) after low-oxygen-pressure synthesis. This impurity can be controlled by changing the synthesis temperature, which makes this material promising for spintronic applications. We have studied this material by magnetic, transport and thermoelectric experiments. The electrical resistivity shows a semiconducting behavior with \( \rho \sim 0.4 \times 10^{-9} \) cm, much lower than Mn- and Co-substituted ZnO. Hall effect measurements show n-type conductivity with mobility \( \sim 10^{3} \) cm\(^2\)/Vs. The n-type conductivity is independent of the presence of ferromagnetic impurities. A high negative Seebeck (-300 \( \mu V/\text{K} \) at 300 K) would make this material suitable for thermoelectric applications if its resistivity could be further reduced. *S. Kolesnik et al., J. Appl. Phys. 95, 2582 (2004). Supported by NSF (DMR-0302617) and the U.S. Department of Education.

4:18PM L12.00008 Anisotropy Lock-in model for the magnetism of (Zn,Co)O, STEFANO SANVITO, Trinity College Dublin — An explanation for the magnetism of diluted magnetic oxides remains elusive to the present day. Super-exchange is short ranged and leads to anti-ferromagnetic interaction, while double exchange needs unrealistically large charge densities to give room temperature ferromagnetism. Moreover there is growing experimental evidence that free-charges alone are not sufficient for the magnetism, which in turn is driven by intrinsic defects. Supported by density functional theory and Monte Carlo simulations we will present a coherent and complete picture of the magnetism in (Zn,Co)O. We will argue that Co clustering is essential for the magnetism and that a wurtzite CoO phase, difficult to detect by X-ray, is responsible for most of the magnetic signal. In this picture, strongly compensated CoO clusters with random anisotropy fields mimic the hysteresis loops often observed experimentally and attributed to long-range ferromagnetic interaction.

4:30PM L12.00009 Enhanced Magnetism in Fe-Doped TiO2 Anatase Nanorods1, YI DING, L. H. LEWIS, WEI-QIANG HAN, Brookhaven National Laboratory — In addition to the applied interest concerning dilute magnetic semiconductors, ferromagnetism in d oxides is of fundamental interest in understanding the interaction character between magnetic impurities in insulating systems. We report here simultaneous ferromagnetism and enhanced Pauli Paramagnetism in TiO2 anatase nanorods doped with nominal 0.5 at% Fe, synthesized by a hydrothermal route followed by low-temperature heating in air. The resultant nanorods are \( \sim 20 \) nm in width and several hundreds nanometers in length. Transmission electron microscopy (TEM) reveals that the Fe concentration ranges from 0.3 at% - 0.8 at% within the nanorods. No evidence of pure iron nanoparticles in the sample is detected with TEM or with synchrotron diffraction. SQUID magnetometry performed in the temperature range 10 K \( \leq T \leq 800 \) K in fields up to 1 T show clear ferromagnetic behavior, suggesting that Fe leads to an enhancement of ferromagnetism. Decomposition of magnetization curves reveals that the nanorods possess Pauli paramagnetism that is over 100 times larger than that of pure bulk anatase TiO2 as well as ferromagnetism that persists to temperatures slightly above 800 K. It is hypothesized that the Pauli paramagnetism originates from anatase regions with lower Fe doping, while the ferromagnetism originates from regions of higher Fe doping, suggesting a percolative mechanism for ferromagnetism.

1Research performed under the auspices of the U.S. DOE, Office of Basic Energy Sciences under contract No. DE-AC02-98CH1-886.

4:42PM L12.00010 Room temperature ferromagnetism in undoped TiO2 films, P. KHAREL, C. SUKAR, J. THAKUR, C. LAWES, R. NAIR, Wayne State University, V.M. NAIR, University of Michigan, Dearborn, R. SURYANARAYANAN, Universite Paris-Sud, France — We have prepared thin films of undoped TiO2 having rutile and anatase structures, using both spin coating and sputter deposition techniques, on sapphire and quartz substrates. The structural characteristics of the films have been investigated using Raman spectroscopy and transmission electron microscopy (TEM). We found that the annealing condition strongly influences the magnetic properties of the films. When annealed in high vacuum, all films demonstrate room temperature ferromagnetism (FM) whereas air annealed samples show insignificant FM. The ferromagnetic moment in vacuum-annealed samples stored under ambient conditions was not stable, but decayed on a time scale of hours. The sample magnetization was found to depend on the film thickness; the saturation magnetic moment was observed to decrease with increasing film thickness. These results suggest that FM in TiO2 films is mediated by surface oxygen defects. The details of Raman and TEM studies will be presented and the appearance of FM on vacuum annealing will be discussed.
ART A. WOLF, University of Virginia — We have used reactive-biased target-ion beam-sputter deposition to prepare CoTi_{1-x}O_{2} thin films on LaAlO_{3}(100) and SrTiO_{3}(100) substrates for 0.005<=x<=0.06. The influence of the growth parameters on the microstructure, magnetic and transport properties of CoTi_{1-x}O_{2} was systematically investigated. Both pure anatase phase and mixed anatase/rutile phases of TiO_{2} films were obtained by varying the growth conditions and subsequently demonstrated different magnetic and transport properties. All samples show a curie temperature higher than 300 K. The pure anatase CoTi_{1-x}O_{2} thin films have saturated magnetic moments of 1−2 \mu_B/Co at 10 K. The presence of rutile phase seems to greatly enhance the moments at lower temperatures.

5:06PM L12.00012 Observation of ferromagnetic behaviors in doped and undoped TiO_{2} and ZnO , P.V. WADEKAR, Q.Y. CHEN*, P.V. CHINTA, O. LOZANO, Z.H. ZHANG, W.K. CHU, Dept. of Physics and TcSUH, University of Houston, TX, H.W. SEO, Dept. of Physics, University of Arkansas, AR, C.F. SUN, C.C. CHOU, H.D. YANG, L.W. TU, Y.L. CHENG, M.Z. HSU, Dept. of Physics and Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University NSYSU, Kaohsiung, Taiwan — Transition-metal doping has been widely used to produce ferromagnetic oxides such as TiO_{2} and ZnO for use as a diluted magnetic semiconductor. Recently, however, undoped samples were also found to be ferromagnetic. We have studied the ferromagnetic behaviors of ZnO and TiO_{2} single crystals and powders annealed both in vacuum and in flowing oxygen at various temperatures. In order to understand the observed ferromagnetism, we have used X-ray photoemission and electron spin resonance spectroscopy to characterize the possible valance states or chemical bonding variation to study the roles that oxygen vacancies may have played in the occurrence of ferromagnetism. Comparisons on the doped and pure samples will be discussed.* Also with NSYSU

5:18PM L12.00013 Electronic structure of Gd-doped GaN: vacancy-stabilized ferromagnetism , PAUL LARSON, University of Missouri - Department of Physics & Astronomy, SASHI SATPATHY, University of Missouri - Department of Physics — The study of dilute magnetic semiconductors has attracted significant interest recently, especially that of Gd-doped GaN. While experimental evidence for a colossal moment/Gd have been found in the low doping regime, we will focus on the stabilization of ferromagnetism over antiferromagnetism with much better understood 7−8 \mu_B/Gd. Electronic structure calculations have been performed using the LAPW method within the WIEN2k code. Supercell calculations have shown that, in the absence of Ga or N vacancies, the large distance between Gd atoms leads to antiferromagnetism by the superexchange mechanism. Ga and N defects allow for extra electrons or holes to mediate the magnetism between the Gd atoms and stabilize the ferromagnetic state. The degree of vacancies necessary to stabilize ferromagnetism has been approximated within a percolation model. This work is supported by the Air Force Office of Scientific Research.

Tuesday, March 6, 2007 2:30PM - 5:30PM –
Session L13 DMP: Focus Session: Interfacial Ordering Colorado Convention Center Korbel 4C

2:30PM L13.00001 Atomic resolution spectroscopic imaging of electronic phenomena in oxide interfaces , M. VARELA, H. M. CHRISTEN, H. N. LEE, D. H. KIM, L. PETIT, T. C. SCHULTHESS, J. TAO, A. R. LUPINI, S. J. PENNYCOOK, Oak Ridge National Laboratory, W. LUO, S. T. PANTELIDES, Vanderbilt University, J. GARCIA-BARRIOCANAL, C. LEON, J. SANTAMARIA, Universidad Complutense, Spain — Electron energy loss spectroscopy in the STEM is a powerful tool to study the structure, chemistry and electronic properties of oxides with atomic resolution, in real space. In perovskites the O 2p bands and the transition metal 3d bands are very close to the Fermi level so the electronic properties can be probed by studying the fine structure on the O K edge and the transition metal L edge. Column-by-column EELS reveals direct information about the unique phenomena going on in oxide interfaces. For example, in superconducting/ferromagnetic YBa_{2}Cu_{3}O_{7}/La_{0.7}Ca_{0.3}MnO_{3} superlattices significant transfer of electrons from the manganite into the superconductor is found over nanometric length scales. But quite different phenomena occur in other manganite interfaces such as LaMnO_{3}/SrTiO_{3}. In this talk both experiments and first principles calculations with simulations of the ELNES will be discussed. Sponsored by the Office of Basic Energy Sciences, Div. of Materials Sciences and Engineering, US DOE under contract DE-AC05-00OR22725 with ORNL managed by UT-Battelle LLC, by the ORNL LDRD Program and by the ORNL-ORISE Postdoctoral Program.

2:42PM L13.00002 Magnetic and electronic properties of complex oxide interfaces , WEIDONG LUO, MARIA VARELA, STEPHEN J. PENNYCOOK, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — Interfaces between complex oxide materials based on perovskite oxides can have novel physical properties. We study the magnetic and electronic properties of La_{0.67}Ca_{0.33}O_{3}/YBa_{2}Cu_{3}O_{7}/La_{0.7}Ca_{0.3}MnO_{3} (LCMO/YBCO) superlattices using first-principles density-functional theory (DFT). The energetics of several types of magnetic (spin) configurations of Mn ions near the LCMO/YBCO interface have been calculated using the DFT approach. Their magnetic and electronic properties have been explored and compared to the properties of bulk materials. These results are compared to recent experimental observation of suppressed magnetization at the LCMO/YBCO interface. We will also discuss the possibility of charge transfer across the interface, as suggested by recent experimental results from local electron energy-loss spectroscopy (EELS). This research was sponsored by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC, and by the McMinn Endowment at Vanderbilt University.

2:54PM L13.00003 Modified doping at cuprate / lanthanum manganite interfaces , JACOBO SAN-TAMARIA, J. GARCIA BARRIOCANAL, A. RIVERA, C. LEON, GFMC, Fac. Fisicas. U. Complutense, Madrid Spain, M. VARELA, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA, S.J. PENNYCOOK, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA, Z. SEFRIOUI, GFMC, Fac. Fisicas. U. Complutense, Madrid Spain — Oxygen heterostructures allow combining materials with similar structure but with very different ground states, which may compete at the interface to yield novel behaviors and functionalities. We explore the YBa_{2}Cu_{3}O_{7} (YBCO) / La_{0.7}Ca_{0.3}MnO_{3} (LCMO) interface in thin film heterostructures. For x=0.3 the manganite is ferromagnetic which causes a strong depression of the superconductivity at the YBCO side. There is also a depression of the ferromagnetic moment at the interface suggesting electron transfer from the manganite into the YBCO. This is confirmed from superlattices alternating YBCO and LaMnO_{3} (LMO), an A-type AF insulator. While for thin LMO layers (<6 unit cells) there is little effect on YBCO superconductivity, thicker LMO layers result in reduced Tc values and induced ferromagnetism at the interface, thus providing a firm indication of charge transfer. The occurrence of charge transfer over length scales much longer than the Thomas Fermi screening length (1 nm) is a novel behavior which, we hope, will stimulate future theoretical studies. Work supported by CICYT MAT2005 06024 C02-02.
3:06PM L13.00004 Interaction between magnetism and superconductivity in \(\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3/\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}\) multilayers\(^1\), T. HU, H. XIAO, C. C. ALMASAN, Department of Physics, Kent State University, Kent, OH 44242, USA, C. VISANI, Z. SEFRIoui, J. SANTAMARIA, GMFC, Departamento Física Aplicada III, Universidad Complutense de Madrid, 28040 Madrid, Spain — Angular dependent resistivity measurements were performed on \(\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3/\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}\) (LCMO/YBCO) heterostructures below and above the superconducting transition temperature \(T_c \approx 90\) K in different applied magnetic field. Besides the conventional intrinsic anisotropic magnetoresistance (AMR) present above \(T_c\), we observe another anisotropic magnetoresistance, which only arises below \(T_c\) and increases significantly with decreasing temperature. Also, the proximity-induced resistance, which appears in the LCMO layer, displays a spectacular increase at \(T_c\) and then decreases significantly with decreasing temperature, persisting down to the lowest measured \(T\) of 72 K. This anomalous AMR and the proximity-induced resistance in the LCMO layer could be due to the triplet component of the superconducting condensation which penetrates into the ferromagnet over a long distance.

\(^1\)This research was supported by the National Science Foundation under Grant No. DMR-0406471 at KSU and MCYT MAT 2005-06024 at U. Complutense de Madrid.

3:18PM L13.00005 Magnetic anisotropy and vortex dynamics in LCMO/YBCO heterostructures\(^1\), H. SRIKANTH, N.A. FREY, University of South Florida, C. VISANI, J. SANTAMARIA, Universidad Complutense, Madrid — Interplay of ferromagnetism and superconductivity in heterostructures of highly spin polarized CMR oxides and cuprate superconductors, is of topical interest. We have used a sensitive radio-frequency (RF) resonant method based on a tunnel-diode oscillator (TDO) to simultaneously probe the dynamic magnetic susceptibility and the vortex penetration depth in well characterized sputtered bi-layers (LCMO/YBCO) and tri-layers (LCMO/YBCO/LCMO), grown on STO substrates with the thickness of LCMO and YBCO being 40 u.c. and 15 u.c., respectively. Transverse susceptibility in the normal state shows distinct peaks associated with the anisotropy fields in LCMO. In the superconducting state, complex coupled response is observed with the region just below \(T_c\) dominated by flux flow in a vortex liquid state. Experimental results with various field orientations are reported and analyzed in the context of proximity effect, spin diffusion, flux penetration and dissipation in the presence of geometrical barriers. Overall, our work demonstrates the effectiveness of RF experiments in probing the magnetization and vortex dynamics in these systems.

\(^1\)Work at USF supported by DAAD19-03-1-0277 and at UCM by CICYT- MAT 2005-06024- C02-01.

3:30PM L13.00006 Magnetism at the interface between ferromagnetic and superconducting oxides,\(^1\), JAK CHAKHALIAN, University of Arkansas — Atomically controlled interfaces between two materials can give rise to novel physical phenomena and functionalities not exhibited by either of the constituent materials alone. Modern synthesis methods have yielded high-quality heterostructures of oxide materials with competing order parameters. Although magnetic correlations at the interface are expected to be important in determining the macroscopic properties of such nanosystems, a quantitative determination of the interfacial magnetic structure in oxides has thus far been very limited. Here we examine superlattices composed of the half-metallic ferromagnet \(\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3\) and the high-temperature superconductor \(\text{YBa}_2\text{Cu}_3\text{O}_7\) by core-level absorption spectroscopy with circularly polarized x-rays and by diffuse neutron reflectometry. The resulting data yield microscopic insight into the interplay of spin and orbital degrees of freedom at the interface. The data also reveal an extensive rearrangement of the magnetic domain structure at the superconducting transition temperature. The combination of techniques establishes an incisive probe of the interplay between competing electronic order parameters in oxide heterostructures. J. Chakhalian, J. W. Freeland, G. Srajer, J. Strempfer, G. Khaulilllin, J. C. Cezar, T. Charlton, R. Dalgliesh, C. Bernhard, G. Cristiani, H.-U. Habermeier and B. Keimer, “Magnetism at the interface between ferromagnetic and superconducting oxides,” Nature Physics, v.2., 244 (2006).

\(^1\)Work at Argonne National Laboratory is supported by the United States Department of Energy, Office of Basic Energy Sciences, under contract No. W-31-109-ENG-38.

4:06PM L13.00007 Interface Magnetic Order in \(\text{LaFeO}_3/\text{LaCrO}_3\) and \(\text{LaFeO}_3/\text{LaAl}_{1-x}\text{MnO}_3\) Superlattices, H.N. LEE, Materials Science and Technology Division, Oak Ridge National Laboratory, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, G. KHALJILLIN, B. KEIMER, Max Planck Institute for Solid State Research, Stuttgart, J. CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville — Creation of sharp interfaces between strongly correlated electron systems can result in novel states at the boundary. Here we present our work using element-resolved x-ray probes to study the magnetic order in \(\text{LaFeO}_3/\text{LaCrO}_3\) and \(\text{LaFeO}_3/\text{LaAl}_{1-x}\text{MnO}_3\) superlattices. Using pulsed laser deposition with RHEED control, (111) and (100) oriented ultra-thin superlattices were grown with layer thicknesses of 1 to 9 unit cells. In the bulk \(\text{LaFeO}_3\) and \(\text{LaCrO}_3\) are antiferromagnetic while \(\text{LaAl}_{1-x}\text{MnO}_3\) is ferromagnetic. At the interface of (111) oriented \(\text{LaFeO}_3/\text{LaAl}_{1-x}\text{MnO}_3\) superlattices we find clear sign of large net magnetic moment on both Mn and Fe even at moderate fields. For the \(\text{LFO}/\text{LCO}\) case, the (111) case displays small net magnetic moment in both layers while the (100) oriented samples shows no clear sign of net magnetic moment even at fields up to 5T. Research sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC.

4:18PM L13.00008 Study of an interface between a double-exchange and a band insulator system, IVAN GONZALEZ, ROGER MELKO, Oak Ridge National Laboratory, JOSE RIERA, Universidad Nacional de Rosario, Argentina, ELBIO DAGOTTO, Oak Ridge National Laboratory, and University of Tennessee — We study the heterostructure consisting of a double-exchange system and a band insulator using DMRG techniques. By changing some parameters of the system, such as the doping, we can sample the different phases of the bulk double-exchange material and observe how the properties at the interface change. We analyze the interesting phenomena appearing in the system such as the behavior of the charge distribution, and the nature of the state immediately at the interface itself. Transport through the heterostructure is also discussed.

4:30PM L13.00009 Doping the interface of Mott-Insulator heterostructures, WEI-CHENG LEE, TAMI PEREG-BARNEA, ALLAN MACDONALD, Department of Physics, The University of Texas at Austin — Recent rapid progress in techniques for layer-by-layer growth of transition metal oxides is making new types of heterostructures available. Previous studies have demonstrated interesting charge transfer and band bending effects near interfaces between Mott insulators and band insulators [1] and between polar and non-polar insulators [2]. We propose [3] interesting effects at several different classes of heterojunctions between ABO3 perovskites based on a single-band Hubbard model studied with several different approximate treatments of electron-electron interactions. Some potentially interesting material combinations will be discussed.

\[1\] A. Ohtomo, etc., Nature 419, 378 (2002).
\[2\] N. Nakagawa, etc., Nature Materials 5, 204 (2006).
4:42PM L13.00010 Polar Kerr effect of epitaxial magnetite thin films in the visible and near infrared spectral region. JI CHENG, GEORGE STERBINSKY, BRUCE WESSELS, Northwestern University — Magnetite thin films are of interest for spin polarized injection and magneto-electric devices. The polar magneto-optical Kerr effect (MOKE) and optical absorption were measured on epitaxial films over the visible and near infrared spectral region at room temperature. Magnetite thin films on magnesium oxide, strontium titanate, barium titanate and spinel substrates were deposited by molecular beam epitaxy using molecular oxygen and iron. A complex MOKE spectrum was measured over the spectral range of 1.5 to 3.0 eV. A negative transition was observed at 1.6 eV and a positive transition at 2.7 eV. These were previously attributed to intervalence charge transfer and intersublattice charge transfer transitions. The detailed spectrum was dependent upon the substrate suggesting strain may be playing a role. Using MOKE magnetometry the coercive field was measured. The coercive field of the epitaxial film varied from 370 gauss for films deposited on MgO to 620 gauss for films deposited on barium titanate.

4:54PM L13.00011 Epitaxial CoFe$_2$O$_4$ (111)-based multilayers for spin filter applicationsootnote{Supported by MIT-France program and CNANO Ile de France.}, ANA RAMOS, JEAN-BAPTISTE MOUSSY, MARTINE GAUTIER-SOYER, CEA-Saclay, France — Efficient spin filtering at room temperature has high potential for ultra sensitive detectors and spin injection into semiconductors, leading to the growth of spin-based devices. We investigate the interaction of spin filter CoFe$_2$O$_4$(111) epitaxial tunnel barriers with Co and Fe$_3$O$_4$ electrodes in light of their possible application at room temperature. The question of the exchange coupling which often prohibits the independent switching between a magnetic tunnel barrier and its magnetic electrode is addressed, as is the difference between an oxide-metal and oxide/oxide system. Our study of the magnetic reversal in the CoFe$_2$O$_4$/Co and CoFe$_2$O$_4$/Fe$_3$O$_4$ bilayers, supported by a detailed structural and chemical analysis of the samples and their interfaces, clearly evidences the effect of a metallic or an oxide interface. An unusual exchange spring magnet behavior arises in the case of the CoFe$_2$O$_4$/Fe$_3$O$_4$ samples due to the superexchange interactions found in these ferrimagnetic oxides. This unique exchange phenomenon at the oxide-oxide interface ultimately leads to a barrier/electrode system that switches independently without the necessity of a non-magnetic spacer.

5:06PM L13.00012 Electron leakage and double-exchange ferromagnetism at a prototype metal-insulator interface: CaRuO$_3$/CaMnO$_3$ootnote{This work was supported in part by the U. S. Department of Energy under Grant No. DE-FC02-00ER45818.}, BIRABAR NANDA, Department of Physics, University of Missouri, Columbia (MO) — Density-functional studies of the electronic structure of a prototype interface between a paramagnetic metal and an antiferromagnetic insulator (CaRuO$_3$/CaMnO$_3$) reveal how magnetism near the interface can be modified by the leaked electrons from the metallic to the insulating side. These electrons mediate a ferromagnetic interaction between the interface Mn moments via Anderson-Hasegawa double-exchange, which competes with the already existing antiferromagnetic superexchange, resulting in an interfacial ferromagnetic layer. Electron penetration beyond the first layer is insufficient to alter the bulk antiferromagnetism. We argue that a canted state in the first layer is possible, consistent with earlier magnetic measurements on this system.

3:06PM L25.00002 Understanding electronic properties at organic/silicon interfaces from first principles. LEEOR KRONIK, Weizmann Institute of Science — Organic/inorganic interfaces often possess properties that are significantly different from those of the organic molecules and the inorganic substrate that comprise them, due to both inter- molecular and molecule-substrate interactions. In this talk, I show how we explore such electronic effects using first principles calculations of prototypical silicon/organic interfaces. I focus on dipole depolarization effects, demonstrated for benzene derivatives on Si(111), and on interface-induced gap states, demonstrated on alkyl chains on Si (111). By comparing the results to both experiment and phenomenological models, we rationalize these effects and predict their manifestation in a range of organic electronic structures and devices.

4:42PM L25.00003 Ferromagnetism in a Porphyrin-based Organic Semiconductor. J. MORENO, M.A. MAJIDI, W.A. SCHWALM, University of North Dakota, R.S. FISHMAN, Oak Ridge National Lab — Current efforts in growing supramolecular quasi two-dimensional magnetic organic semiconductors, such as porphyrin-based or bimetallic oxalates materials, have not been followed by close theoretical studies of their magnetic properties. Interplay between experimental and theoretical approaches is needed to increase their ferromagnetic transition temperatures, which are still quite low. Our aim is to contribute to the theoretical effort by studying a simplified model of a two-dimensional array of magnetic ions embedded in a porphyrin matrix. Since the distance between the local moments is very large their magnetic couplings are mediated by the metal-like extended pi-orbitals. Therefore, our approach is based on a Double-Exchange Hamiltonian with effective hopping between magnetic ions derived from Hückel model. We solve this model using the Dynamical Mean Field Approximation (DMFA) including several ions on the local site. In order to predict the optimal magnetic properties, we calculate the ferromagnetic transition temperature, magnetization and susceptibility for a range of parameters.
3:54PM L25.00004 Self-Assembly of Magnetic Molecules on GaN(0001)  SAW W. HLA, DANDA P. ACHARYA, VIOLETA IANCU, ERDONG LU, ARTHUR R. SMITH, Ohio University — Self-assembled clusters of TBrPP-Co molecules are formed on a freshly grown nitrogen polar GaN(0001) surface. The structural and electronic properties of the molecular clusters are then studied by using a scanning tunneling microscopy and spectroscopy at low-temperature (4.6 K) under an ultra-high-vacuum condition. The TBrPP-Co molecule has a spin-active cobalt atom caged at the center of porphyrin unit and four bromo-phenyl groups are attached to its four corners. On GaN(0001), the molecules bind the surface through the bromo-phenyl units and form a saddle conformation, in which the central part of the molecule is bent by lifting the two pyrrole units of the porphyrin macrocycle. Within the self-assembled molecular clusters on this surface, the molecules are aligned either parallel or 90 degree rotated to each other. This molecule-substrate system may be useful for spintronic applications. This work is supported by NSF-NIRT grant number DMR 0304314.

4:06PM L25.00005 Atomic and Electronic Structure of a Novel Two-Dimensional Molecular Magnet System  ANTHONY CARUSO, North Dakota State University, TREVOR TYSON, NIIT, DOUGLAS SCHULZ, North Dakota State University, WOLFGANG CALIEBIE, Hasy Lab, DESSY — Molecular magnet systems show much promise to replace standard metals and metal oxide systems in a broad range of application due to the comparative simplicity of processing. Understanding the coupling of the spins in these systems is important to determine their full range of applicability. We have studied the local atomic and electronic structure of a recently synthesized Mn carboxylate system which forms two-dimensional interconnected rings. To understand the spin interactions, the local atomic and electronic structure about the Mn sites was investigated by x-ray absorption spectroscopy and high resolution x-ray emission spectroscopy. The valence and spin configuration are described. Comparisons are made between the coupling of Mn sites via the oxygen atom with standard magnetic oxide systems such as the magnetites.

4:18PM L25.00006 Growth and electronic structure of tetracyanoethylene on noble metals studied by scanning tunneling microscopy  DANIEL WEGNER, RYAN YAMACHIKI, YAYU WANG, Department of Physics, University of California at Berkeley, BART BARTLETT, JEFF LONG, Department of Chemistry, University of California at Berkeley, MIKE CROMMIE, Department of Physics, University of California at Berkeley — Tetracyanoethylene (TCNE, C₄(N-CN)₂) is a π-electron acceptor with a very strong electron affinity that easily forms charge-transfer complexes with other organic molecules and metals. We have performed STM and STS of isolated TCNE molecules and ordered sub-monolayer coverages on noble-metal surfaces in order to study the competition between intermolecule and molecule-substrate interactions, and the impact this might have on film-growth and electronic structure. HOMO and LUMO peaks were observed for single TCNE molecules on Ag and Au substrates using STS, but not for Cu substrates which react more strongly with TCNE. The spatial distribution of the TCNE HOMO, as observed in dl/dv maps, fits well with DFT calculations and shows that TCNE is in a negatively charged state on these metal substrates. dl/dv maps of ordered TCNE arrays indicate that neighboring TCNE molecules interact strongly with each other in some cases.

4:30PM L25.00007 Strong electron-phonon interaction in e-e correlated molecular systems1  YURI DAHNOVSKY, Department of Physics & Astronomy, University of Wyoming, Laramie, WY 82071-3905 — Molecular systems (molecules) with strong electron-phonon interaction are described in terms of the Green functions. In the case of the strong e-ph interaction a general scheme that includes of the Dyson equations for the electron and phonon Green functions, is not productive. Hence, the different methodology is developed where the unitary transformation (that included both electron and phonon subsystems) is used. In this case the Dyson equation for the electron Green function is not valid any longer. Different approximations are proposed. The developed approach is extremely important for electron transfer reactions without single electron transfer assumption. It can be also used in the transport in molecular junction devices.

4:42PM L25.00008 Electron Spin Relaxation in Hole Polarons States of Conjugated Porphyrin Arrays  PAUL J. ANGIOLILLO, Saint Joseph’s University, PAUL R. FRAIL, University of Pennsylvania, NORA GRANETO, DEVLIN MURDOCK, Saint Joseph’s University, MICHAEL J. THERIEN, University of Pennsylvania — It has been previously demonstrated that stable hole-polaron states may be produced in a family of highly π-conjugated (porphinato)Zn(II) in which the monomeric units are bridged by ethyne linkages. Furthermore, EPR results verify that hole delocalization or incoherent hopping occur over substantial distances (∼ 7.5 nm) along a single conjugated backbone. The electron spin relaxation times in traditional conducting materials are on the order of picoseconds. Preliminary data gleaned from progressive microwave saturation will show that electron spin relaxation times in these materials are on the order of 1 μs at 295 K in both solution and in film architectures and moreover are relatively insensitive to oligomer length with distances spanning 1.4 to 7.5 nm. Since hopping rates have been observed to be on the order of 10¹¹ Hz, it is possible then for spin memory of the hole polaron to be retained during its migratory process.

4:54PM L25.00009 Spin states and their relaxation in transition-metalorganic self-assembled molecules1  ZHI-GANG YU, SRI International, 333 Ravenswood Avenue, Menlo Park, CA 94025 — The coexistence of spins localized on transition-metal ions and mobile charges on the π-conjugated ligands in transition-metalorganic self-assembled molecules (TMSAMs) makes these molecules attractive for molecular spintronic devices and quantum computing. We present our theoretical results on the spin states localized on the transition-metal ion in a TMSAM using both the first-principles approaches and the ligand-field theory. Then we construct a spin Hamiltonian to calculate spin lifetimes and identify the dominant spin relaxation mechanisms in the molecule. We also discuss the relation between the spin states on the transition-metal ion and the charge transport along the π-conjugated ligand in the molecule.

5:06PM L25.00010 Low Temperature STM Investigation of Molecular Kondo Effect  GAYANI PERERA, VIOLETA IANCU, SAW-WAI HLA, Ohio University — We investigate site-dependent Kondo effect on TBrPP-Co molecules on a Cu(111) surface at 4.6 K using scanning tunneling microscopy and spectroscopy [1]. The TBrPP-Co molecule has a spin-active cobalt atom caged at the center of porphyrin unit and four bromo-phenyl groups are attached to its four corners. On Cu(111), the molecules can anchor on the surface with either planar or saddle conformation [2]. For the current study, we choose only planar type molecules, in which the porphyrin unit is lying parallel to the surface and the molecule binds through the surface via four bromo-phenyl units as well as central porphyrin unit. The Kondo temperature of 170 K is measured above the cobalt atom location, i.e. at the center of the molecule. The observed Kondo effect is caused by spin-electron coupling between the cobalt atom of the molecule and the free electrons from the surface [2,3]. We find that the Kondo effect observed here is contributed from both surface and bulk states of Cu(111). This work is supported by the US Department of Energy Basic Energy Sciences grant no. DE-FG02-02ER46012. [1] G. Perera, V. Iancu, Luis G.G. Días da Silva, S.E. Ulloa, and S.-W. Hla. Submitted. [2] V. Iancu, A. Deshpande, and S.-W. Hla, Nano Lett. 6 (2006) 820-823. [3] V. Iancu, A. Deshpande, and S.-W. Hla, Phys. Rev. Lett. (2006) in press.

Tuesday, March 6, 2007 2:30PM - 5:30PM  Session L28 DMP: Focus Session: Carbon Nanotube Optics IV  Colorado Convention Center 302
2:30PM L28.00001 Probing Non-equilibrium Phonon Dynamics in Carbon Nanotubes by Time-Resolved Raman Spectroscopy. DAOLUA SONG, FENG WANG, TONY F. HEINZ. Columbia University — In this paper we present a direct determination by femtosecond pump-probe laser spectroscopy of the lifetime of zone-center optical phonons in semiconducting single-walled carbon nanotubes. The non-equilibrium phonon population was created by the rapid relaxation following ultrafast optical excitation of the E_{22} transition of a suspension of isolated HipCO nanotubes. As a probe of the phonon population, we made use of antiStokes Raman scattering from G mode. From the variation of the Raman signal with pump-probe delay, we deduced a phonon lifetime around 1 ps. The relation between the measured population lifetime and Raman linewidth will be considered, as will be the implication of this result for the existence of non-equilibrium phonon population in nanotubes carrying high current densities.

2:42PM L28.00002 One Dimensional Exciton Diffusion on Semiconducting Nanotubes using Time Resolved Photoabsorption Spectroscopy. R. M. RUSSO, D.E. LUZZI, E.J. MELE. University of Pennsylvania — We extend our recently reported analysis of the population relaxation of optically excited states on semiconducting carbon nanotubes to study the spectral shifts of their photoabsorption spectra. Highly excited tubes show a long time 1/\sqrt{t} decay of their photobleaching spectra which is well described by a one dimensional diffusion limited two body population relaxation. We find that the absorption spectra also show time-dependent spectral shifts with respect to the ground state absorption spectra. The spectral shifts are of order 10 nm and history dependent: two tubes prepared from different initial excitation densities but evolving to the same instantaneous excitation density show different lineshapes and spectral shifts. These features are analyzed by a model for the distribution of exciton separations produced in a diffusing population. The model provides an excellent parameter free description of the lineshape, and gives an estimate of the experimental exciton diffusion constant.

2:54PM L28.00003 Tracing exciton formation and relaxation in (6,5)-enriched single walled carbon nanotubes with sub-10 fs resolution. LARRY LÜER, CNR/INFM ULTRAS Politecnico di Milano, CALOGERO SCIASCIA, Dipartimento di Fisica, Politecnico di Milano, CHRISTOPH GADERMAIER, JARED CROCHET, TOBIAS HERTEL, Vanderbilt University, Nashville, TN — We perform pump and probe spectroscopy on (6,5) enriched single walled carbon nanotubes using broadband visible pulses of 7 fs duration. Apart from the photogeneration of the E22 exciton, we find a delayed channel which is operative at higher pump intensities during the first 20 fs after photoexcitation. It results in i) a saturation of the maximum population of the E22 exciton and ii) a strong retardation of the relaxation kinetics of E22 into E11, that cannot be accounted for by considering regeneration of E22 states by annihilation of E11 states. We suggest free carrier recombination as origin of the delayed E22 formation channel. The G mode oscillation of the nanotubes is traced via coherent oscillations as function of probe wavelength. It exhibits an abrupt phase jump at the maximum of the E22 absorption band, clearly demonstrating the oscillation of the E22 transition energy exerted by the G mode vibrational distortion. Mapping the oscillatory amplitudes against probe wavelength allows us to separate oscillations in the ground state from those in the excited state.

3:06PM L28.00004 Time-Domain Ab Initio Studies of Phonon-Induced Relaxation of Electronic Excitations in Carbon Nanotubes. OLEG PREZHDHO, University of Washington — Electron-phonon interactions in carbon nanotubes (CNT) determine response times of optical switches and logic gates, the extent of heating and energy loss in CNT wires and field-effect transistors, and even a mechanism for CNT superconductivity. Numerous time-resolved experiments have revealed intriguing features of the electron-phonon relaxation in CNTs in response to external stimuli. We report the ab initio studies of the relaxation performed in real-time, directly mimicking the experimental data. The results reveal a number of unexpected features of the relaxation processes, including the differences between the intraband relaxation and electron-hole recombination, the photoexcitation energy dependence of the relaxation, the importance of defects, the dependence on the excitation intensity, and a detailed role of active phonon modes.

3:42PM L28.00005 Exciton-Polariton Dynamics in Carbon Nanotubes. IGOR BONDAREV, North Carolina Central University — This work addresses theoretically the nonlinear response of phonon-coupled excitons in carbon nanotubes to an external electromagnetic field. The photon Green’s function approach developed recently to quantize the electromagnetic field in the presence of quasi-1D absorbing bodies is being used to study the dynamics of phonon-coupled excitonic states interacting with the surface photonic modes excited by the external electromagnetic field in semiconducting carbon nanotubes. The formation of the new elementary excitations, exciton-polaritons, representing the eigenstates of the full photon-matter Hamiltonian has been studied for small-diameter nanotubes under strong exciton-photon coupling. Time-resolved simulations have been performed of the coherent exciton-polariton dynamics with the exciton-phonon interactions taken into account. The criteria for the coherent control of the excitonic states population in optically excited carbon nanotubes have been formulated.

3:54PM L28.00006 Photoinduced transient mid-infrared absorption in single-walled carbon nanotubes. YOICHI MURAKAMI, Rice University, University of Tokyo, WILLIAM RICE, JUNICHIRO KONO, Rice University — We have performed optical pump - mid-infrared (MIR) probe spectroscopy on single-walled carbon nanotubes (SWNTs). The second excitonic absorption band (E_{22}) of (6,5) SWNTs was resonantly excited and the resulting photoinduced absorption was monitored in the MIR range (3.5 – 5.5 μm) in a time range up to several hundred ps. Carragianen films containing individualized CoMoCAT SWNTs formed on sapphire substrates were used for the measurement. This sample is optically transparent in the ~3.5 – 6 μm region, where the transition of E_{11} excitons from the lowest dark state (1g) to the second bright state (2u) is expected to be observed. Our preliminary data shows the existence of photoinduced absorption in the investigated range. The origin of the observed transient absorption will be discussed.

4:06PM L28.00007 The Graphenic Bicontinuum Provides a Unified Analytical Treatment of Lattice Dynamics in Carbon Nanostructures. CRISTIANO NISOLI, VINCENT CRESPI, Department of Physics, Penn State University, ERIC MCKENSTURM, Department of Mechanics and Nuclear Engineering, Penn State University — A two-field bi-continuum model for the vibrational dynamics of graphene and carbon nanotubes describes a wealth of phenomena absent in a traditional continuum, including optical phonons, the high wave-vector nonlinearity of the acoustic branches, and even the hexagonal graphic Brillouin zone. Since it includes all the degrees of freedom of the honeycomb lattice, the model provides a complete description of the important electromechanical effects such as strain-induced gap opening or gap-induced phonon softening. The bi-continuum provides a unified framework for understanding and extending a previously disparate accumulation of analytical and computational results on deformations and vibrations in carbon nanostructures.

4:30PM L28.00009 Electron-phonon renormalization effects in the ARPES spectra of doped graphene: a first principles approach, FRANCESCO MAURI, MATTEO CALANDRA, IMPMC, Université Paris 6 — Recent experimental investigations of the hole excitations in graphene [1], bilayer graphene [2] and graphite [3] by angular resolved photoemission indicated the occurrence of kink structures in the band dispersions and in the lifetime of hole excitations. These kinks have been attributed to electron-phonon coupling effects. In this work we calculate the effect of electron-phonon scattering on the angular resolved photoemission spectra (ARPES) of graphene as a function of doping. We use electron-phonon coupling parameters derived from density functional theory calculations. We compare our results for the quasiparticle dispersion and for the lifetime of the electrons and holes with those obtained from ARPES.

1 A. Bostwick et al., cond-mat/0609600
3 S. Zhou et al. cond-mat/0609028

4:42PM L28.00010 Anisotropic electron-phonon coupling in doped graphene, JESSICA MCCHESNEY, Montana State University, ALS, AARON BOSTWICK, Advanced Light Source- LBNL, TAI-SUKE OHTA, Fritz Haber Institute, THOMAS SEYLLER, Université Erlangen-Nuernberg — The effects of doping single layer graphene are investigated by mapping the valence band in the vicinity of EF using angle-resolved photoemission spectroscopy (ARPES). The carrier concentration was varied from 0.04 – 1.05 electrons per unit cell with the deposition of Ca and K at low temperatures. As the doping increases there is an enhancement of the electron-phonon coupling along certain high symmetry directions. Changes in electron-phonon coupling parameter, lambda, shows that the systems goes through a transition from the weak-coupling regime to the strong-coupling regime.

4:54PM L28.00011 Thermo-Plasma-Polariton within Scaling Theory of Single-Layer Graphene, OSKAR VAFEK, Florida State U. - NHMFL — Electrodynamics of single-layer graphene is studied in the scaling regime. At any finite temperature, there is a weakly damped collective thermo-plasma-polariton mode whose dispersion and wavelength dependent damping is determined analytically. The electric and magnetic fields associated with this mode decay exponentially in the direction perpendicular to the graphene layer, but unlike the surface plasma polaron modes of metals, the decay length and the mode frequency are strongly temperature dependent. This may lead to new ways of generation and manipulation of these modes.

5:06PM L28.00012 Theory of resonant multi phonon Raman scattering in graphene monolayers, DENIS BASKO, IGOR ALEINER, Columbia University, Physics Department — The Raman spectrum of graphene consists of distinct narrow peaks corresponding to different optical phonon branches as well as their overtones [1]. We show how the relative intensities of the overtone peaks encode information about relative strengths of different inelastic scattering processes electrons are subject to. In particular, assuming that the most important processes are electron-phonon and electron-electron scattering, it is shown that one can deduce their relative interaction strengths from the Raman spectra. [1] A. C. Ferrari et al., Phys. Rev. Lett. 97, 187401 (2006); A. Gupta et al., cond-mat/0606593; D. Graf et al., cond-mat/0607562.

5:18PM L28.00013 Extracting optical properties of individual or few layers of graphite oxide sheets on surfaces by developing simple optical approaches1, INHWA JUNG, RICHARD PINDER, DIMITRY DIKIN, SASHA STANKOVICH, SUPINDA WATCHAROTONE, RODNEY RUOFF, Northwestern University — An optical method for extracting optical properties of individual or few layers of graphite oxide sheets is presented. The substrate consists of a dielectric layer of controlled thickness on semiconducting silicon. The intensity ratio between reflected light from the material and the substrate can be optimized through choice of the optical properties and the thickness of the individual or few layers of graphite oxide sheets on surfaces by developing simple optical approaches. We find that one can extract these optical properties which might otherwise not be discerned through “standard” optical microscopy.

1We appreciate support from the Naval Research Laboratory #N00173-04-2-C003/P00005, and from the NASA URETI “BIMat” Institute (#NCC-1-02037).

Tuesday, March 6, 2007 2:30PM - 5:30PM — Session L39 FIAP DMP: Focus Session: Hydrogen Storage II

2:30PM L39.00010 NMR Studies of the Li-Mg-N-H Phases. , ROBERT BOWMAN, Jet Propulsion laboratory, J. W. REITER, J. G. KULLECK, JPL, S.-J. HWANG, Caltech, WEIFANG LUO, SNL — Solid state NMR including magic-angle-spinning (MAS) and cross-polarization (CP) MAS experiments have been used to characterize various amide and imide phases containing Li, Mg, MAS-NMR spectra for the 6Li, 7Li, and 15N nuclei have been obtained to improve understanding on formation, processing, and degradation behavior. Only limited information could be obtained from the proton and 13C MAS-NMR spectra due to large dipolar interactions and small chemical shifts. However, more success was obtained from the 6Li and 15N nuclei although their very long spin-lattice relaxation times did impact signal acquisition times. For example, three distinct 6Li peaks were resolved from LiNH2 phases that were clearly separated from the LiH secondary phase in these samples. While the 15N spectra for LiNH2 phase in isotopically enriched samples exhibited only a single peak at least three distinct 15N peaks were observed from the similarly enriched Mg amide samples. These differences will be related to crystal structures. The NMR spectra also revealed very little motion in these hydrides upon to nearly 500 K.
Electronic Structure and Energetics of the Quaternary Hydride Li$_3$BN$_3$H$_{10}$

JAN HERBST, LOUIS HECTOR JR., GM Research and Development Center, Warren, MI 48090-9055 — Li$_3$BN$_3$H$_{10}$ has been synthesized recently from LiNH$_2$/LiBH$_4$ mixtures and its crystal structure determined. We have calculated the electronic structure of this complex hydride and investigated its thermodynamic stability and decomposition energetics. We find that its enthalpy of formation is $\sim 708$ kJ/mole with respect to the elemental constituents and $\sim 6$ kJ/mole relative to a 3:1 molar LiNH$_2$/LiBH$_4$ mixture, in qualitative agreement with experiment. Reaction enthalpies computed for several decomposition pathways suggest

$$\text{Li}_4\text{BN}_3\text{H}_{10} \rightarrow \text{Li}_2\text{BN}_2 + \frac{1}{2}\text{Li}_2\text{NH} + \frac{3}{2}\text{NH}_3 + 4\text{H}_2$$

as the likely dehydridding route.

Tetragonal I4$_1$/amd Crystal Structure of Li$_3$BN$_2$ from Dehydrogenated Li-B-N-H

FREDERICK PINKERTON, JAN HERBST, General Motors Research and Development Center, Warren, MI — We have determined the crystal structure of Li$_3$BN$_2$ formed by dehydrogenation of Li$_3$BN$_3$H$_{10}$ from powder x-ray diffraction (XRD) data using the Rietveld method. XRD measurements indicate unambiguously that this Li$_3$BN$_2$ polymorph is distinct from any of the previously reported Li$_3$BN$_2$ phases. We find a body-centered tetragonal I4$_1$/amd structure (space group No. 141 in the International Tables for X-ray Crystallography) with $a = 6.60$ Å and $c = 10.35$ Å. The structure features tightly coordinated, nearly linear N–B–N units with 1.3 - 1.4 Å B–N bond lengths suggesting covalently bonded (BN)$_2$+$^-$ anions. In situ temperature-dependent XRD showed that the body-centered tetragonal Li$_3$BN$_2$ phase was present both at elevated temperature during dehydrogenation and after cooling to room temperature. We also describe the results of first principles theoretical modeling of the body-centered tetragonal Li$_3$BN$_2$ polymorph as well as the tetragonal P4$_{2}$$\overline{1}$2$_2$ and monoclinic P2$_1$/c Li$_3$BN$_2$ structures previously reported. We obtained excellent agreement between the theoretically calculated I4$_1$/amd Li$_3$BN$_2$ lattice constants and atomic positions and those obtained experimentally from XRD. The approximate enthalpy of formation of the I4$_1$/amd Li$_3$BN$_2$ phase is $\Delta H = -495$ kJ/mole-formula unit.

Ab-initio Investigations of Li and Mg Amide-Imide Systems for Hydrogen Storage

TAKAO TSUMURAYA, TATSUYA SHISHIDOU, TAMIO OGUCHI. Hiroshima University — Reversible hydrogen storage in light-elemental materials has been recognized as one of the most practical approaches for on-board application. Lithium nitride Li$_3$N can reversibly store large amount of hydrogen in the two-step reversible reaction composed of lithium amide LiNH$_2$ and imide Li$_2$NH[1]. Quite recently, in an effort to reach further performance, several types of magnesium substitutions in Li-N-H system have been investigated. For instance, Leng et al. have examined a composite material made by ball milling of 3:8 molar mixture of magnesium amide Mg(NH)$_2$$_2$ and lithium hydride LiH[2]. The hydrogenation and dehydrogenation reaction mechanism and fundamental properties of these hydrides still remain as a matter to be investigated. In particular, crystal structures of some metal imides such as Li$_2$NH, MgNH and Li$_2$Mg(NH)$_2$ are not fully determined yet. In this paper, we discuss structural stability and heats of formation of these hydrides from first-principles calculations based on the all-electron FLAPW method. [1] P. Chen Z. Xiong, J. Luo, J. Lin and K.L. Tan, Nature 420, 302 (2002). [2] H. Y. Leng, T. Ichikawa, S. Hino, N. Hanada, S. Isobe and H. Fujii, J. Phys. Chem. B 108, 8763 (2004).

First-principles investigation of the Li-Mg-N-H system

ZHU MA, YAN WANG, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology — The Li-Mg-N-H system has been identified as a promising hydrogen storage material due to its moderate operation conditions as well as the high capacity and reversibility. The Li-Mg mixed imide is reported to have disordered cation or cation-vacancy arrangements at room temperature and above. We present our first-principles investigation to study the crystal structure of Li$_2$Mg(NH)$_2$ using total energy calculations within the density functional theory. A series of ordered low-energy configurations are identified. Specific local orders are found in the cation-vacancy arrangement, shedding light on the experimental disordered structure models. A possible ordered phase at lower temperature is proposed based on our calculation. Furthermore, the reaction energetics and phase stability involved in this system are discussed.

Ab-initio kinetics and thermodynamics studies of ammonia-borane for hydrogen storage

CAETANO R. MIRANDA, GERBRAND CEDER, Massachusetts Institute of Technology — Ammonia-borane (BH$_3$NH$_3$) is a promising chemical hydrogen storage material given its high gravimetric and volumetric properties. However, the ammonia-borane (AB) thermal hydrogen release is not very efficient, being mainly limited by the kinetics of hydrogenation. Using ab initio calculations, we have investigated the thermodynamics and kinetics of hydrogen release on AB by calculating the free energies of the H$_2$ release reactions for different possible decomposition products. Our results indicate that AB regeneration through the ammonia-borane polymeric and borazine-cyclotriborazine cycles is very unlikely due to the strong exothermic character of the reactions. The kinetics of hydrogen release is further investigated with the recently developed metadynamics method. This method allows us to calculate the multidimensional free energy surface of hydrogen release on AB. Our simulations reveal the atomistic mechanism of hydrogenation and provide the free energies barriers and transition states involved in inter and intramolecule H$_2$ release on AB.

This research was supported by the DOE under Contract DE-FG02-05ER46253

Ab-initio kinetics and thermodynamics studies of ammonia-borane for hydrogen storage

PARDINVESTIGATION of the Direct Hydrogenation of Aluminum to Alane in Supercritical Fluids

CRAIG JENSEN, University of Hawaii, SEAN MCGRADY, REYNA AYABE, University of Hawaii, BEN REDDY, University of New Brunswick — Alane, AlH$_3$ has many of the properties that are requisite for materials to be considered viable for onboard hydrogen storage applications. Most notably, it contains 10.1 wt% hydrogen and undergoes dehydrogenation at appreciable rates at temperatures below 100$^\circ$C. However, the very low, $\leq 6$ kJ/mol, enthalpy of dehydrogenation of AlH$_3$ prohibits subsequent re-hydrogenation through standard gas-solid techniques except at very high pressures or very low temperatures. The extremely low solubility of gaseous H$_2$ in conventional organic solvents also vitiates a solution-based approach. Re-hydrogenation of Al using a supercritical fluid potentially offers a workable approach since the fluid can act as a solvent, at the same time remaining completely miscible with permanent gases like hydrogen. Recently, it has been found that mixtures of NaH and Al can be hydrogenated to sodium alane, NaAlH$_4$ under modest pressures and temperatures in supercritical fluids. We have now extended these studies to the hydrogenation of Al to AlH$_3$. The results of these studies and experimental details will be reported.

Stability Studies of Aluminum Hydride

XIA TANG, BRUCE LAUBE, United Technologies Research Center, DONALD ANTON, Savannah River National Laboratory, SON-JONG HWANG, Div. of Chem. and Chem. Eng., California Institute of Technology, ROBERT BOWMAN, Jet Propulsion Laboratory, CALIFORNIA INSTITUTE OF TECHNOLOGY COLLABORATION, JET PROPULSION LABORATORY, CALIFORNIA INSTITUTE OF TECHNOLOGY COLLABORATION — Aluminum hydride has attracted research attention recently as a promising hydrogen storage material due to its high gravimetric, volumetric storage capacity and very low enthalpy. AlH$_3$ forms several phases, all of which are sensitive to moisture. In this study, the discharge kinetics of a stabilized form of alpha aluminum hydride newly synthesized was evaluated. Its desorption kinetics were measured in the temperature range of 60-120$^\circ$C at one atmosphere of hydrogen pressure. The material was stable at ambient temperature and no significant dehydrogenation was observed at 60$^\circ$C after 70 hours. Approximately 10 wt% hydrogen was rapidly (quantify in wt%/min.) released at 100$^\circ$C with no additional catalization. The activation energy for desorption was measured at 97.0 KJ/mole H$_2$. The surface and bulk characterization methods Auger, SEM, XRD, and solid state NMR were used to investigate the mechanism of stabilization.
4:06PM L39.00009 Atomic Simulations of Alane Phase Transformations and Dehydrogenation Mechanisms. SUSANNE OPALKA, United Technologies Research Center, PAUL Saxe, Materials Design, Inc., OLE MARTIN LOVVVIK, University of Oslo — Density functional theory atomic ground state, molecular dynamics, and direct method lattice dynamic simulations were used to mechanistically probe phase transformations between the various crystallographically refined α, α′, β, and γ AlH₃ phases. Lattice dynamic predictions of the AlH₃ structures provided an ideal test case for systematically accessing the accuracy of the vibrational thermodynamic property contributions with the harmonic approximation. The predicted transformation pathways involved coordinated tilting and rotation mechanisms, similar to that observed in perovskite structures. Further simulations were conducted to elucidate the mechanism for α AlH₃ phase decomposition to the Al and H₂ products and to identify probable barriers to reversible rehydrogenation.

4:18PM L39.00010 Trapped H₂ in AlH₃. MARK CONRADI, LASITHA SENADHEERA, ERIK CARL, T.M. IVANCIC, Washington U., Physics, R.C. BOWMAN, JR., JPL, S.J. HWANG, Caltech, Chemical Eng., T.J. UDOVIC, NIST, Gaithersburg — Trapped molecular hydrogen has been discussed for years in H-storage systems such as NaAlH₄. Here we report proton NMR and neutron vibration spectroscopy (NVS) evidence for H₂ in AlH₃ samples. In static sample NMR, a sharp line appears on top of the broad AlH₃ solid signal. MAS further sharpens this line and identifies it as H₂ by its chemical shift. Upon cooling, the line broadens and disappears near 20K, confirming the H₂ identification. NVS reports energy-gain peaks at the H₂ rotational energy (J=1 to 0).

4:30PM L39.00011 Inelastic Neutron Scattering Investigation of Ti-doped NaAlH₄. MONIKA HARTL, ALICE ACATRINEI, LUKE DAEMEN, Los Alamos National Laboratory — Complex hydrides (i.e. alanes (AlH₄)−) or borates (BH₄)−) are widely investigated as hydrogen storage materials. They have lower formation energy than simple metal hydrides and usually higher hydrogen to metal ratio. However, kinetics and performance still represent the main challenge for the actual application of these materials as hydrogen storage materials. The use of transition metal dopants such as Ti, Fe, Zr can improve the hydrogen exchange capability and hydrogen storage capability of a complex metal hydride significantly. However, a satisfactory explanation how and why certain dopants work best with certain complex metal hydrides has not yet been given. We choose sodium aluminium hydride NaAlH₄ doped with various amount of titanium (precursor: TiCl₄) for our research on the mechanism of doping. Incoherent inelastic neutron spectroscopy is a well-suited tool to look at hydride (H−) in the material and the changes of the hydride in the material upon addition of dopants. Possible changes in the lattice of the "host material" NaAlH₄ are observed by X-ray diffraction.

4:42PM L39.00012 Hydrogen-related defects and the role of Ti in NaAlH₄. AMRA PELES, CHRIS VAN DE WALLE, University of California Santa Barbara — Titanium-doped sodium alanate is a promising storage material; however, the mechanism of the enhancement in (de)hydrogenation rates induced by Ti has remained unresolved. We performed a comprehensive investigation of hydrogen vacancies and interstitials, which play an important role in the (de)hydrogenation processes. Interestingly, these highly mobile defects cause large rearrangements of the surrounding lattice, and they are always charged; their formation energy therefore depends on the Fermi level. Our investigations show that the Ti-induced modification of the Fermi level increases the defect concentrations, thus explaining the improved kinetics. These novel insights may prompt a reexamination of the role of transition-metal impurities in alanes and related materials, and lead to the design of storage materials with improved characteristics.

5:06PM L39.00014 Thermodynamic properties of LiAlH₄ from first-principle calculations. XUEZHI KE, CHANGFENG CHEN, Department of Physics, University of Nevada, Las Vegas, NV 89154-4002, USA — The potential hydrogen-storage materials of LiAlH₄ and Li₃AlH₆ have been studied by using density functional theory (at GGA level), and harmonic phonon approximation. The thermodynamic properties of these materials have been studied. We present here the first-principles molecular dynamics results for NaAlH₄, one of the promising and most extensively studied candidates for hydrogen storage. We analyze proton transport in the presence of a variety of low-energy defects and surfaces, and we discuss possible candidates for the key mechanisms of dehydrogenation in the material. The results are presented in terms of the structural phase transition to α-Na₃AlH₆.

5:18PM L39.00015 Hydrogen adsorption studies in micro-size cobalt dots. ALBERTO. CABRERA, C.P. ROMERO, J.I. AVILA, E. CISTERNAS, G.B. CABRERA, Departamento de Fisica, P. Universidad Catolica de Chile, K. TEMST, M.J. VAN BAEL, Laboratorium Voor Vaste-Sttofysica en Magnetisme, K.U. Leuven, Belgium — Hydrogen desorption curves were obtained from a sample composed of square arrangement of Co dots with average diameter of 4.4 microns, separated by a distance of 11.6 microns. A macroscopic sample of Co dots grown on a 2.5x2.5 cm Si substrate was made by standard lithographic techniques and used in these experiments. Thermal programmed desorption (TPD) was performed under ultra-high vacuum conditions. Hydrogen TPD curves were obtained from a 1x1 cm sample of Co dots, Co films and Co foils for comparison. The hydrogen TPD curves peaked at 425 K and have decreasing intensity from the Co foils to the Co dots and to the Co films. A desorption energy of 27 Kcal/mol was obtained for the Co dots suggesting that hydrogen is adsorbed on an hcp or fcc hollow site of the Co dot crystalline structure.
2:30PM L44.00001 Image potential and molecular conductance, IVAN OLEJNIK, MORTKO KOZHUSHNER, University of South Florida — The image potential plays an important role in condensed matter physics including tunneling phenomena at surfaces, but its role in molecular conductance has not been thoroughly investigated. We discuss the influence of the image potential on molecular conductance. It is known that the predominant mechanism of conductance in relatively long organic molecules is resonant tunneling, i.e. the current between electrodes is due to resonant transfer of electrons via the resonant levels of the negative molecular ion (electron states) or/and the levels of positive molecular ion (hole states). Both the energies and wave functions of these resonant states are influenced by the dynamic image potential of the tunneling electron due to the presence of both electrodes. The physics of the image potential is governed by the relative balance between the plasmon energy of electrodes and the band width of the molecular resonant states. In particular, the image potential may lower the resonant electronic levels by as much as 1 eV or raise the resonant hole levels by the same amount. We will discuss interesting phenomena associated with image potential including possible diode effects in symmetric molecules.

2:42PM L44.00002 Real-space pseudopotential method for charge and spin transport properties of nanoscale junctions. LINGZHU KONG, University of Minnesota, JAMES R. CHELIKOWSKY, University of Texas at Austin, JEFFREY B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, University of California, Berkeley & Lawrence Berkeley National Laboratory — We present an ab initio method for the electronic transport of nano-scale junctions under finite bias. Our method is based on density functional theory using real space pseudopotentials. The scattering wave function is obtained by solving a set of linear equations with a sparse coefficient matrix. Our method does not require a matrix inversion. We apply the method to Na or Mg atomic point contacts coupled to two planar electrodes, and good agreement with previous work is obtained. We also extend this study and examine spin-dependent transport in select magnetic atomic point contacts, where trends in magnetoresistance are examined as a function of junction bias, magnetic moment, and electronic coupling.

1Supported by the National Science Foundation under DMR-0551195 and DMR04-39768, and by the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760. Portions of this work were performed at the Molecular Foundry, which is supported by DOE.


Densiy functional calculations of nanoscale conductance, Connie Chang, Max Koentopp, Kieron Burke, and Roberto Car, in prep.

3:06PM L44.00004 Is Density Functional Theory adequate for quantum transport?1, KIERON BURKE, UC Irvine — Density functional calculations for the electronic conductance of single molecules attached to leads are now common. I’ll examine the methodology from a rigorous point of view, discussing where it can be expected to work, and where it should fail. When molecules are weakly coupled to leads, local and gradient-corrected approximations fail, as the Kohn-Sham levels are misaligned. In the weak bias regime, XC corrections to the current are missed by the standard methodology. Finally, I will compare and contrast several new methodologies that go beyond the present standard approach of applying the Landauer formula to ground-state DFT. Self-interaction errors in density functional calculations of electronic transport, C. Toher, A. Filippetti, S. Sanvito, and K. Burke, Phys. Rev. Lett. 95, 146402 (2005).


Density functional calculations of nanoscale conductance, Connie Chang, Max Koentopp, Kieron Burke, and Roberto Car, in prep.

1Supported by DOE.

3:42PM L44.00005 Ab initio calculation of transmission and I-V curve for π-stacked polythiophene layers sandwiched between gold electrodes. SERGEY FALEEV, FRANCOIS LEONARD, Sandia National Laboratories, MARK VAN SCHILFGAARDE, Arizona State University — We have applied an implementation of recently developed [Faleev et al. PRB 71, 195422 (2005)] non-equilibrium Green’s Function method in framework of the tight-binding LMTO approach in its atomic sphere approximation to calculate the transmission function and I-V curves of π-stacked polythiophene layers sandwiched between Au(111) electrodes. Our approach is a fully ab initio all-electron approach that treats the central region and electrodes on equal footing. To the best of our knowledge, this is first application of an ab initio approach to calculation of transport properties of multiple polymer layers arranged parallel to the metal surface, as opposed to previously studied systems of a small molecule or oligomer attached at both ends to the electrodes. We found that for a number of layers L > 1, an increasingly pronounced dip in the transmission function is formed at energies Er > 0.5 eV, reflecting the semiconductor nature of a polythiophene multilayer film. The zero-bias conductance of the film exhibits large-L asymptotic behavior σ ≈ Ge−exp(−1.2(L−1)), starting with L ≈ 6 that can be seen as a thickness of the thin polythiophene film at which a metal-semiconductor transition occurs. For L = 1, the current depends linearly on applied voltage, while at L > 1, current is non-linear, reflecting strong bias and energy dependence of the transmission function.

3:54PM L44.00006 First Principles Simulation of STM Image and Spectroscopy, YU ZHU, McGill University, HONG GUO TEAM — In this talk, we shall present a framework for simulating STM images and transport spectroscopy based on density functional theory (DFT) carried out within nonequilibrium Green’s function approach (NEGF). In our model, the STM tip and the sample are treated together on equal footing within the self-consistent NEGF-DFT formalism, in contrast to the usual practice where electronic structure of the tip and sample are calculated separately. The NEGF-DFT formalism allows one to do STM simulation whether the STM tip is far (weak coupling) or close (strong coupling) to the sample. The main implementation issues of this STM simulation tool will be discussed and several examples will be given.

4:06PM L44.00007 Electron correlations in transport through molecular junctions: Coulomb blockade and hysteresis in the I-V characteristics of a model system. CATALIN D. SPATARU, Columbia University, MARK S. HYBERTSEN, Brookhaven National Lab, ANDREW MILLIS, Columbia University, STEVEN G. LOUIE, University of California at Berkeley — Electron-electron interaction effects can play a very important role in explaining the mechanism of charge transport in molecular junctions. We use a simple tight-binding model to describe the leads and the electron-ion interaction inside the molecule. The electron-electron interaction inside the molecule is treated at the Hartree-Fock level. We study the model as a function of the number of sites in the molecule and the alignment of molecular energy levels relative to the average chemical potential in the leads. This model captures important phenomena such as the Coulomb blockade. We find that depending on the gate voltage and applied bias, there can be more than one Hartree-Fock steady-state solution for the system, which may give rise to a hysteresis in the I-V characteristics.
4:18PM L44.00008 Quantum quasi-steady states in current transport\(^1\). ROBERTO D’AGOSTA, University of California - San Diego, MICHAEL ŻWOLAIK, California Institute of Technology, MASSIMILIANO DI VENTRA, University of California - San Diego — We investigate quasi-steady state solutions to transport in quantum systems by finding states which at some time minimize the change in density throughout all space and have a given current density flowing from one part of the system to another [1]. Contrary to classical dynamics, in a quantum mechanical system there are many states with a given energy and particle number which satisfy this minimization criterion. Taking as an example spinless fermions on a one-dimensional lattice, we explicitly show the phase space of a class of quasi-steady states. We also discuss the possibility of coherent and incoherent mixing of these steady state solutions leading to a new type of noise in quantum transport. [1] M. Di Ventra and T.N. Todorov J. Phys. Cond. Matt. 16, 8025 (2004).

\(^1\)Work supported in part by NSF and DOE.

4:30PM L44.00009 DC conductance of long molecular chains\(^1\). ROBERTO CAR, EMIL PRODAN, Princeton University — Inspired by the work of Kamenev and Kohn, we obtained a general and formally exact expression for the 2-terminal dc conductance of linear molecular structures, within the framework of Time Dependent Current-Density Functional Theory. In this talk we focus on the adiabatic conductance. For linear molecular chains, both insulating and metallic, we derive exact and asymptotic analytic expressions for the conductance. For insulating chains, for example, not only do we get the exponentially decaying factors, but also the coefficients in front of these factors, which are highly dependent on the contacts. The results are based on the analytic structure of the bands and a compact expression for the Green’s functions. Applications will also be presented.

\(^1\)NSF PCCM, DOE.

4:42PM L44.00010 Nonequilibrium Electron Transport in Mott Insulators. K. A. AL-HASSANIEH, F. HEIDRICH-MEISNER, I. GONZALEZ, E. DAGOTTO, Oak Ridge National Laboratory, Oak Ridge TN, and University of Tennessee, Knoxville TN 37381, USA, A. E. FEIGUIN, Microsoft Project Q, The University of California at Santa Barbara, Santa Barbara, CA 93106, USA, M. J. ROZENBERG, Departamento de Física, FCEN, Universidad de Buenos Aires, Ciudad Universitaria Pabellón I, Buenos Aires 1428, Argentina — We study the nonequilibrium transport properties of a Mott insulator using a recently developed time-dependent DMRG procedure to study conductances [1]. As a setup, we use a Hubbard chain connected to two ideal leads. We find a simple functional form of the I-V characteristics, and a universal functional dependence of the current on the electric field and the Mott gap. A mechanism of transport is described based on these results. The properties of the conducting phase induced by a strong electric field are also studied. We compare these properties to those of the doped phase. We also compare the Mott insulator to the band insulator case and discuss the similarities and differences [2].


4:54PM L44.00011 Conductance, surface traps and passivation in doped Silicon Nanowires. MARIVI FERNANDEZ-SERRA, CECAM ENS-Lyon, CHRISTOPHE ADESSI, LPMCN Universite Lyon 1, XAVIER BLASE, CNRS et LPMCN Universite Lyon 1 — By means of ab initio total energy and conductance calculations within the Landauer Formalism we investigate the structural, electronic and transport properties of doped silicon nanowires (SiNWs). We find that impurities always segregate at the surface of unpassivated wires, reducing dramatically the conductance of the surface states. Upon passivation, we show that for wires as large as a few nanometers in diameter, a large proportion of dopants will be trapped and electrically neutralized at surface dangling bond defects, significantly reducing the density of carriers. Impurities located in the core of the wire induce a strong resonant backscattering at the impurity bound state energies. Surface dangling bond defects have hardly any direct effect on conductance. Upon surface trapping, impurities become transparent to transport, as they are both electrically inactive and do not induce any resonant backscattering.


5:06PM L44.00012 Low-Temperature Nonequilibrium Transport through Multi-pathway Single-Molecule-Transistor Systems as Which-way Effect Detector. HAIZHOU LU, ZUO-ZI CHEN, RONG LU, Center for Advanced Study, Tsinghua University, Beijing 100084, China, BANG-FEN ZHU, Center for Advanced Study, Tsinghua University, Beijing 100084, China and Department of Physics, Tsinghua University, Beijing 100084, China — We theoretically investigate the electronic transport through an AB-ring with a quantum dot (QD) embedded and a double-quantum-dot (DQQ) interferometer. The QDs in both structures are coupled to a vibrational mode by electron-phonon interaction. With the help of Non-equilibrium Green function formalism and an improved independent boson model approximation, low-temperature bias-induced phonon-assisted sidebands are resolved. Electrons can tunnel via the phonon sidebands, pure electronic levels, or directly from one lead to the other. For DQQ interferometer, electrons tunneling via two dots must emit the same number of the identical phonons to interfere with each other. Emitting different numbers of phonons would make the two pathways distinguishable, thus destroys the coherence between two pathways. Therefore this system could act as an intrinsic which-way effect detector in energy space. For the AB-ring model, the which-way effect does not apply since the direct lead-lead tunneling alone do not we get the exponentially decaying factors, but also the coefficients in front of these factors, which are highly dependent on the contacts. The results are based on the analytic structure of the bands and a compact expression for the Green’s functions. Applications will also be presented.

5:18PM L44.00013 Observation of tribo-induced melting of an asperity contact with STM-QCM\(^1\). JACQUELINE KRIM, SANG-MIN LEE, DOUG L. IRVING, CLIFF W. PADGETT, DON W. BRENNER, North Carolina State University — Heating, energy dissipation and melting at the interface of a nanoscale sliding contact can trigger a broad range of interfacial physical and chemical processes. A fundamental understanding of these processes is largely lacking, however, because they occur at buried interfaces that are extremely difficult to characterize during sliding. In the arena of nanotechnology, heating, energy dissipation and conversion issues are integral to successful device design, construction and operation. Particularly compelling is the fact that any frictional heat produced is available to destroy device function: If any portion melts, the nanoscale device itself is destroyed. We report here on our use of the unique capabilities resulting from combining a scanning tunneling microscope (STM) and a Quartz Crystal Microbalance (QCM) to characterize the melting of a buried sliding interface between a tungsten tip and an indium overlayer. An analytic heat transport model supports the conclusion of melting arising from tip-surface sliding. These combined results constitute the first compelling evidence for the observation of tribo-induced melting of an asperity contact.

\(^1\)Work supported by NSF and AFOSR Extreme Friction MURI.

Tuesday, March 6, 2007 7:00PM - 8:00PM — Session M46 DMP: DMP Business Meeting  Adam039;s Mark Hotel Plaza Court 7

7:00PM M46.00001 DMP Business Meeting —
8:00AM N8.00001 Engineering superconductors with ab initio methods: the example of LiB.

STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science, Duke University — The identification of novel crystal structures is a fundamental step for predicting new stable compounds in alloys. While performing ab initio data mining of intermetallic compounds [1], we discover a new family of layered metal borides [2], of which MgB$_2$ is one particular element (the new phases are called Metal Sandwich (MS)). Thermodynamic stability and electronic properties of these MS phases are investigated in details, leading to the prediction of a hypothetical novel superconductor MS-LiB [2,3]. Calculations show that the MS phases in the Li-B system exhibit electronic features similar to those of MgB$_2$ [2,3] and CaC$_6$ [4]. Although the predicted critical temperature of LiB is lower than that of MgB$_2$ (references [4] and [5] for MS2-LiB and MS1-LiB, respectively), the peculiarities of MS-LiB in terms of electronic structure, layer arrangements and doping capabilities allow a lot of freedom in the search for higher $T_c$ systems [5]. We acknowledge the San Diego Supercomputer Center for computational resources.


8:36AM N8.00002 Electronic structure of MS2-LiB under hydrostatic pressure.

EDGAR MARTINEZ-GUERRA, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico. ALEKSYE N. KOLMOGOROV, STEFANO CURTAROLO, Duke University, North Carolina, USA. — Recently ab initio calculations have found that the Li-B phase equilibrium diagram has two new phases: MS1 and MS2 [A. Kolmogorov and S. Curtarolo, Phys. Rev. B 73, 180501(R) (2006)]. These two phases are stable enough to compete against known phases. These lithium borides exhibit electronic features similar to those in magnesium diboride and they are expected to be superconductors. In this work, we have studied the structural and electronic properties of the MS2-LiB system under pressure. The calculations were performed using the SIESTA code, with the GGA exchange-correlation functional in the PBE form. We have used numerical atomic orbitals as the basis set for the valence wavefunctions employing a double $\zeta$ approach. We found that the localized vibrational modes associated with the boron atoms provide a significant contribution to the electron-phonon coupling strength and that superconductivity in diamond is crucially linked to the breaking of the lattice periodicity induced by the doping.

This research was partially supported by CONACYT-Mexico under Grant No. 43830-F.

8:48AM N8.00003 Combining the advantages of superconducting MgB2 and CaC6 in one material: suggestions from first-principles calculations.

AMY LIU, Georgetown University, IGOR MAZIN, Naval Research Laboratory — We show that a recently predicted layered phase of lithium monoboride, Li$_2$B$_2$, combines the key mechanism for strong electron-phonon coupling in MgB$_2$ (i.e., interaction of covalent $\sigma$ bands with $\pi$-band stretching modes) with the dominant coupling mechanism in CaC$_6$ (i.e., interaction of free-electron-like interlayer states with soft intercalant modes). Yet, surprisingly, the electron-phonon coupling in Li$_2$B$_2$ is calculated to be weaker than in either MgB$_2$ or CaC$_6$. This is due to the accidental absence of $\pi$ states at the Fermi level in Li$_2$B$_2$. In MgB$_2$, the $\pi$ electrons play an indirect but important role in strengthening the coupling of $\sigma$ electrons. We discuss the use of doping to restore $\pi$ electrons at the Fermi level, which would enhance the coupling and the superconducting $T_c$.

9:00AM N8.00004 The Structural and Physical Properties of the Vacancy Ordered LiBC Phases.

BORÁ KALKAN, EBRU GUNGOR, ENGIN OZDAS, Advanced Materials Research Group, Physics Department, Hacettepe University, Beytepe, Ankara 06800, Turkey — The prediction of superconductivity on the hole doped LixBC system [1] has triggered to particular interest on the synthesis of non-stoichiometric LiBC compounds. However, isolation of a non-stoichiometric phase of the LiBC have not been succeed as a single phase, yet. All of the experimental studies exhibited non-superconductivity in the disordered Li$_x$BC phases. Contrary to the disordered Li$_x$BC phases synthesized in the literature [2], non-stoichiometric Li vacancy ordered phases were obtained in this work. Additionally, the structural analysis with Rietveld refinement in a series of samples identified the stages of the intercalation of Li between the BC layers. The effect of stoichiometry on the physical properties of ordered Li$_x$BC phase was investigated at low temperatures.


9:12AM N8.00005 The Pressure Effect on the Electronic Structure of the Ordered LiBC.

EBRU GUNGOR, ENGIN OZDAS, Advanced Materials Research Group, Physics Department, Hacettepe University, Beytepe, Ankara 06800, Turkey — In this study, the effect of the higher pressures (0-100GPa) on the electronic structure was investigated for an ordered structure of Li$_x$BC phase. And also, the stoichiometric effect was examined by the first principles calculations in terms of the metallic behaviour for the range of $0 \leq x \leq 1$. It was observed that the density of states near the Fermi level decreases depending on the pressure and the energy gap above the Fermi level contracts for the higher pressure values for especially Li$_0$ BC compound predicted as a superconductor [1-3]. DOS is extremely sensitive to the Li stoichiometry and the unit cell volume. The pressure has the different effect on the electronic structure of Li$_x$BC system behaviour for the same pressure range by contrast with the nonstoichiometric LiBC.


FELICIANO GIUSTINO, JONATHAN R. YATES, IVO SOUZA, MARVIN L. COHEN, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — The recent discovery of superconductivity in boron-doped diamond above liquid helium temperature has attracted considerable interest. Theoretical investigations indicate that the superconducting pairing in this material is of the conventional phonon-mediated type. However, the nature of the phonon mechanism involved and the role of the dopants are still controversial issues. In order to elucidate such issues we performed first-principles calculations of the electron-phonon interaction in boron-doped diamond, considering a virtual crystal model and a supercell model which explicitly includes the boron atoms. For each model we calculated the Eliashberg functions with high accuracy by sampling the corresponding Brillouin zone with a million of inequivalent $k$-points. We found that the localized vibrational modes associated with the boron atoms provide a significant contribution to the electron-phonon coupling strength and that superconductivity in diamond is crucially linked to the breaking of the lattice periodicity induced by the doping.

This work was supported by the NSF under Grant No. DMR04-39768, and the U.S. DOE under Contract No. DE-AC02-05CH11231. Computer time was provided by NERSC and NERAC.
9:36AM N8.00007 Critical fields, vortex melting and the irreversibility line in quasi 2D organic superconductors.1, B. KYUNG and A.-M.S. TREMBLAY, Phys. Rev. Lett. are separated by a strong first order transition. The phase diagram gives much insight into the mechanism for d-wave superconductivity. Two predictions are made.

1We acknowledge support from DOE grant #ER46214.

9:48AM N8.00008 Unconventional Metallic States of the Superconducting Layered Organic Charge Transfer Salts , EDDY YUSUF, B. J. POWELL, R. H. MCKENZIE. Physics Department, University of Queensland — We show, by previously analyzing published nuclear magnetic resonance data, that there are large antiferromagnetic (AF) fluctuations above 50 K and a pseudogap below 50 K in the metallic state of κ-(ET)₂Cu[N(CN)₂]Br. We discuss the relationships between the metallic state, the AF Mott insulating state, and the unconventional superconducting state. The AF correlation length is found to be 3.5 ± 2.5 lattice constants at T = 50 K; this places the material between the isotropic triangular lattice and the square lattice. We show that the low temperature regime of the metallic state of κ-(ET)₂Cu[N(CN)₂]Br is not a renormalized Fermi liquid, as has been previously thought. We argue that a pseudogap is responsible for the loss of the density of states in the spin degrees of freedom, seen in NMR data, while that probes of the charge degrees of freedom have a Fermi liquid character in these materials. We compare and contrast our phenomenological description with the predictions of dynamical mean field theory (DMFT) and the resonating valence bond (RVB) theory. Similar spin fluctuations and pseudogap are also found in κ-(ET)₂Cu(N(CN)₂)Cl, fully deuterated κ-(ET)₂Cu[N(CN)₂]Br, and κ-(ET)₂Cu(NCS)₂ suggesting common physics in these salts.

10:00AM N8.00009 Specific heat study of the effect of cooling rate on the superconducting and normal states of κ-(ET)₂Cu[N(CN)₂]Br, ANTONY CARRINGTON, O.J. TAYLOR, C.M.J. ANDREW, University of Bristol, R.W. GIANNETTA, T. OLHEISER, University of Illinois at Urbana-Champaign, J. SCHLUETER, Argonne National Lab. — It is well known that the Tc of κ-(ET)₂Cu[N(CN)₂]Br is dependent on the rate it is cooled in the temperature range 80-60 K. One interpretation of this effect is that rapid cooling introduces disorder which suppresses Tc because of its unconventional nature. Here we present a specific heat study of this effect in both hydrogenated and deuterated samples. We find that not only does Tc depend on the cooling rate, but that the normal-state Sommerfeld coefficient, γ, is strongly suppressed (by up to a factor 2) with rapid cooling. The data indicate that rapid cooling induces macroscopic phase separation between an insulating and metallic / superconducting phase at low temperature. The field dependence of γ for the deuterated sample is highly unusual. As the field is increased it initially increases in a conventional way then suddenly collapses to a small value. We interpret this as evidence for a field induced superconductor-insulator transition.

10:12AM N8.00010 Low temperature penetration depth of κ-(ET)₂Cu[N(CN)₂]Br, J.D. FLETCHER, A. CARRINGTON, H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, BSB 1TL. United Kingdom, R.W. GIANNETTA, Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801, J. SCHLUETER, Chemistry and Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439. — Several experimental results have suggested that the quasi-2D organic metal κ-(ET)₂Cu[N(CN)₂]Br is host to some form of unconventional superconductivity. The presence of gap nodes in the superconducting order parameter should be detectable through power law behavior in the penetration depth at low temperature. The most accurate measurements of the temperature dependent penetration depth to date show a fractional power law, λ ∝ T². However, these measurements were not performed at sufficiently low temperatures to determine whether this was due to the combination of gap nodes and the effects of impurity scattering, or due to an intrinsic form of exotic pair excitation. Using a radio frequency (rf) tunnel diode technique in a dilution fridge we have extended these measurements to T ∼ 75 mK (<0.006 Tc). Special care has been taken to eliminate heating effects at these temperatures due to the presence of the small applied rf field. Data at the lowest temperature are more consistent with a nodal state in the presence of impurities.

10:24AM N8.00011 Mott Transition, Antiferromagnetism, and d-wave Superconductivity in Two-Dimensional Organic Conductors1, A.-M.S. TREMBLAY, BUMSOO KYUNG, Universite de Sherbrooke — We study the Mott transition, antiferromagnetism and superconductivity in layered organic conductors using Cellular Dynamical Mean Field Theory for the frustrated Hubbard model. A d-wave superconducting phase appears between an antiferromagnetic insulator and a metal for t'/t ≥ 0.3 - 0.7, or between a nonmagnetic Mott insulator (spin liquid) and a metal for t'/t ≤ 0.8, in agreement with experiments on layered organic conductors including κ-(ET)₂Cu[N(CN)₂]. These phases are separated by a strong first order transition. The phase diagram gives much insight into the mechanism for d-wave superconductivity. Two predictions are made. B. Kyung and A.-M.S. Tremblay, Phys. Rev. Lett. 97, 046402 (2006)

1Supported by NSERC (Canada), FQRNT (Québec), CFI (Canada), CIAR, Tier I Canada Research Chair Program (A.-M.S.T.)

10:36AM N8.00012 Comparative Studies of Quasi-One-Dimensional Superconductivity in Sc₃Ir₁₀Si₁₀ and Lu₄Ir₁₀Si₁₀, TSUYOSHI TAMEGAI, GUOJI LI, Department of Applied Physics, The University of Tokyo — Compounds with a formula RₛTₐX₁₀ (R=Sc, Y, rare earth elements, T=Co, Ir, Rh, Os, X=Si, Ge) crystallize in Sc₃Cu₈Si₁₀-type structure with Sc-Si chains running along the c-axis. Some of them show superconductivity with relatively high transition temperatures and coexistence of superconductivity and charge-density wave. We have grown high quality single crystals of Sc₃Ir₁₀Si₁₀ and Lu₄Ir₁₀Si₁₀ using the floating-zone method. Thus obtained crystals show superior properties compared with polycrystalline materials, such as higher Tc and Hc₂. Anisotropic superconducting properties in these crystals are studied in detail. The upper critical field shows clear anisotropy, with Hc² || = Hc² ⊥, consistent with the quasi-one-dimensional crystal structure. Both compounds have modest anisotropies with γ(=Hc²/Hc²) = 2.3 for Sc₃Ir₁₀Si₁₀ and γ = 1.6 for Lu₄Ir₁₀Si₁₀. Magnetic penetration depths in Sc₃Ir₁₀Si₁₀ (λ₀ = 900 Å) and λ₀ = 2100 Å) estimated from the magnetic field dependence of the equilibrium magnetization confirm quasi-one-dimensional nature of the superconducting state.

Wednesday, March 7, 2007 8:00AM - 11:00AM –
Session N9 DMP: Superconductivity: Oxide Photoemission II Colorado Convention Center Korbel 1D
8:00AM N9.00001 Theory of Photoemission Line Shape in High Temperature Superconductor Bi$_2$Sr$_2$CaCu$_2$O$_8$+δ via Dipolon Mediated Electron-Electron Pairing Mechanism, RAM SHARMA, University of Illinois at Chicago — Observed photoemission (PE) line shape near (p,0) in superconductor BISCO containing a peak, a dip and a broad feature has been explained naturally by dipolon pair emaning mechanism using temperature dependent expressions [1,2] including all necessary and important electron correlations. The calculated positions of the peak, dip and broad feature agree well with the observed results. The theory predicts the possibility of observing dipolon side bands in PE. Contributions not only from nearest Cu$–$O$_2$ layer but also from all other layers and rows are important. The peak in PE is due to excitation solely of a quasiparticle; the broad feature and dip are due to the excitations of quasiparticles with concomitant O(1,1) and O(1,2) dipolon excitations. In normal state PE [3] of UD, Op and OD samples we have identified these dipolon excitations. Matrix element effects have been considered. [1] R.R. Sharma, Phys. Rev. B 63, 054506 (2001).

8:12AM N9.00002 Van Hove singularity crossing in overdoped superconducting cuprates - effect on superconducting and normal-state properties, JEFFERY L. TALLON, MacDiarmid Institute, JAMES STOREY, Victoria University, TOBIAS FELLMETH, GRANT WILLIAMS, MacDiarmid Institute. We show from modeling the entropy, superfluid density and thermoelectric power using a rigid ARPES-derived dispersion that the crossing of the van Hove singularity (vHs) occurs in Bi$_2$Sr$_2$CaCu$_2$O$_8$ in the heavily overdoped region at a hole concentration of p=0.22 holes per Cu. This concurs with recent results from ARPES measurements. The impact of the vHs crossing on the thermodynamic properties, the Knight shift and susceptibility, transport, optical and superconducting properties is described and shown to account for much of the overall doping dependence of these properties. The only exotic feature that needs to be introduced is the pseudogap showing that much of the physics of HTS materials is unconventional. These insights help us to see that the “lost entropy” of 1kB per doped hole, previously associated with the pseudogap, is just associated with the DOS asymmetry arising from the proximity of the vHs. Remarkable is the insensitivity of the doping dependence of Tc to the singularity in the DOS.

8:24AM N9.00003 Distinct Fermi-momentum dependent energy gaps in deeply underdoped Bi2212, K. TANAKA, W.S. LEE, D.H. LU, Stanford University, A. FUJIMORI, T. FUJII, University of Tokyo, *RISIDIANA, I. TERASAKI, Waseda University, K. FUJITA, M. ISHIKADO, S. UCHIDA, University of Tokyo, D.J. SCALEAPOIN, University of California, Santa Barbara, T.P. DEVEREAUX, University of Waterloo, University of British Columbia, Z. HUSSAIN, Lawrence Berkeley National Laboratory, Z.-X. SHEN, Stanford University — Our recent angle-resolved photoemission spectroscopy study of deeply underdoped cuprate superconductors Bi2Sr2CaCu2O8 (R = Y or Dy) (Bi2212) suggested the presence of two distinct energy gaps exhibiting different doping dependences [1]. One gap, associated with the antinodal region where no coherent peak is observed, increases with underdoping - a behavior known for more than a decade and considered as the general behavior of the gap in the underdoped regime. The other gap, associated with the near nodal regime where a coherent peak can be observed in energy distribution curves (EDCs), does not increase with less doping - a behavior not seen in the single particle spectra before. The theoretical implications of these findings and temperature dependence of the spectra will be discussed. [1] Science, in press. (http://www.sciencemag.org/cgi/content/abstract/11335411)

8:36AM N9.00004 Detail Properties of Band Renormalization Effect of the Bi$_2$Sr$_2$Ca$_2$Cu$_2$O$_{8+δ}$, WEI-SHENG LEE, WORAWAT MEEVESANA, DONGHUI LU, Stanford University, STEVE JOHNSTON, TOMAS DEVEREAUX, University of Waterloo, K. FUJITA, M. ISHIKADO, S. UCHIDA, University of Tokyo, D.J. SCALEAPOIN, University of California, Santa Barbara, T.P. DEVEREAUX, University of Waterloo, University of British Columbia. In Bi$_2$Sr$_2$Ca$_2$Cu$_2$O$_{8+δ}$, we have performed high-resolution ANGLE RESOLVED PHOTOEMISSION studies of the BSCCO family of superconductors. This higher resolution, in both energy and position, allows us to discern details of the superconducting gap that are not visible at lower resolution. The pseudogap shows up as a broad dip. We observe distinct peak-dip-hump structures above and below Tc. These features are due to the excitation of quasiparticles along the nodal and antinodal directions. Above Tc, we observe a sharp peak and a broad dip at the same energy. We speculate that the pseudogap state competes with superconductivity by diminishing spectral weight in the superconducting antinode. We generate a rich superconductivity and doping induced phenomena. Simulations based on electron-phonon interaction will also be discussed in comparison to our data.

8:48AM N9.00005 Evidence for two energy scales in the superconducting state of optimally doped (Bi,Pb)$_2$(Sr,La)$_2$CuO$_{6+δ}$, TAKESHI KONDO, TSUNEHIRO TAKEUCHI, SYUNSUKE TSUDA, SHIK SHIN, ADAM KAMINSKI, Ames Lab. and Dept. of Physics and Astronomy, Iowa State University — We use angle-resolved photoemission spectroscopy (ARPES) to investigate the properties of energy gap(s) in the optimally doped (Bi,Pb)$_2$(Sr,La)$_2$CuO$_{6+δ}$ (Bi2201). We find significant differences in the momentum- and temperature-dependence of the pseudogap and superconducting gap suggesting that these gaps have two separate energy scales. The ARPES spectra slightly off the node have a sharp peak with a small gap below Tc, which closes at Tc. Around the antinode, the broad spectra with a large energy gap of ~40meV are observed above and below Tc. The spectral shape and the gap size around the antinod are almost unchanged across Tc, indicating that the pseudogap state coexists with superconducting state below Tc, and it dominates the character of ARPES spectra around antinode. We speculate that the pseudogap state competes with superconductivity by diminishing spectral weight in the superconducting antinode.

9:00AM N9.00006 Laser-ARPES studies of BSCO-BASED cuprate superconductors, J.F. DOUGLAS, J.D. KORALEK, Z. SUN, University of Colorado, N.C. PLUMB, Q. WANG, T.J. REBER, J.D. GRIFFITH, University of Colorado, Y. AITSAK, K. OKA, H. EISAI, AIST, TSUKUBA, JAPAN, ZHI-XUN SHEN, Stanford University — The last decade has witnessed a dramatic improvement of the angle-resolved photoemission spectroscopy (ARPES) technique in terms of energy and momentum resolution. In turn, has resulted in a number of new findings on the electronic structure of high-Tc cuprate superconductors, particularly the identification of many-body effects. In this talk, we will present results on the electronic structure of high-Tc superconductors measured from our new ARPES system based on VUV laser, realized by frequency doubling from a non-linear optical crystal KBBF. The laser-based ARPES system has ultra-high energy resolution, high photon flux, and a potential to enhance bulk sensitivity.

9:12AM N9.00007 VUV Laser-Based ARPES on Electronic Structure of High Temperature Superconductors XINGJIANG ZHUO, GUODONG LIU, WENTAO ZHANG, HANYUN LIU, LIN ZHAO, JINGQIAO MENG, XIAOLI DONG, National Laboratory for Superconductivity, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, Z.Y. XU, G.L. WANG, H.B. ZHANG, Y. ZHOU, Key Laboratory of Optical Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, C.T. CHEN, Y. ZHU, G.C. ZHANG, X.H. WEN, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100080, China, G.D. GU, Physics Department, Brookhaven National Laboratory, Upton, New York 11973 — The last decade has witnessed a dramatic improvement of the angle-resolved photoemission spectroscopy (ARPES) technique in terms of energy and momentum resolution. This in turn has resulted in a number of new findings on the electronic structure of high-Tc cuprate superconductors, particularly the identification of many-body effects. In this talk, we will present results on the electronic structure of high-Tc superconductors measured from our new ARPES system based on VUV laser, realized by frequency doubling from a non-linear optical crystal KBBF. The laser-based ARPES system has ultra-high energy resolution, high photon flux, and a potential to enhance bulk sensitivity.
9:24AM N9.00008 Protected nodes and the collapse of the Fermi arcs in high \( T_c \) cuprates, AMIT KANIGEL, U. CHATTERJEE, Department of Physics, University of Illinois at Chicago, M. RANDERIA, Department of Physics, Ohio State University, Columbus, M.R. NORMAN, Materials Science Division, Argonne National Laboratory, S. SOUMA, M. SHI, Department of Physics, University of Illinois at Chicago, Z.Z. LI, Laboratoire de Physique des Solides, Université Paris-Sud, H. RAFFY, Laboratoire de Physique des Solides, Université Paris-Sud, France, J.C. CAMPUZANO, Department of Physics, University of Illinois at Chicago — Angle resolved photoemission studies on underdoped samples of \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) reveal that the superconducting gap’s magnitude and anisotropy remain unchanged up to \( T_c \). Above \( T_c \), the nodes of the \( d-wave \) gap abruptly expand into finite length Fermi arcs. As this change occurs within the resistive width of the transition, we argue that the Fermi arcs are not simply thermally broadened nodes, but rather a unique signature of the pseudogap phase. This is in contrast to BCS theory, which predicts a gap with fixed anisotropy that changes with temperature and disappears above \( T_c \).

9:36AM N9.00009 The Shrinking “Fermi Arc” in Cuprates, LIJUN ZHU, C. M. VARMAN, University of California, Riverside — The angle-resolved photoemission spectroscopy (ARPES) on cuprates in the pseudogap region reveal an extraordinary topological transition in which the ground state changes from one with a usual Fermi surface to one with four Fermi points. We argue that such a state is not possible without some symmetry breaking which allows interference between one-particle basis states which is normally forbidden. We also show that the experimental results are quasi-two-dimensional given without any free parameters by a theory and discuss the implications of the results.

9:48AM N9.00010 Electronic structure of \( \text{La}_{2−x}\text{Sr}_x\text{NiO}_4 \) in the charge-order regime, MARCO PAPAGNO, JEFF GRAF, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, TAKAO SASAGAWA, Department of Physics, Stanford University, Stanford, California, T. KAKESITA, CREST, Japan Science and Technology Agency, Saitama 332-0012, Japan, ALESSANDRA LANZARA, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley & Department of Physics, University California Berkeley, California — We report high resolution angle resolved photoemission spectroscopy (ARPES) studies of the electronic structure of \( \text{La}_{2−x}\text{Sr}_x\text{NiO}_4 \), a doped antiferromagnet compound in which the added holes order in diagonal stripes at 45° to the Ni-O bond. A detailed study of the electronic structure as a function of momentum, temperature and doping is presented. Evidence of the one-dimensional character of the electronic structure and its evolution with doping will be presented. Similarities and differences of the electronic structure of the nickelates with the stripe phase of other correlated materials as high temperature superconductors and colossal magneto resistance manganesites will be discussed.

10:00AM N9.00011 Nature of the quasiparticle remnant in \( \text{La}_{2−x}\text{Sr}_x\text{CuO}_4 \) (LSCO), A. BANSIL, S. SAHRAKORPI, R.S. MARKIEWICZ, Northeastern U., M. LINDROOS, V. ARPAINEN, Tampere UT, Finland, X.J. ZHOU, Stanford U., T. YOSHIDA, U. of Tokyo, Kashiwi, W.L. YANG, Stanford U., T. KAKESITA, Superconductivity Research Laboratory, ISTEC, Tokyo, H. EISAKI, National Institute of Advanced Industrial Science and Technology, Tsukuba, S. UCHIDA, U. of Tokyo, Bunkyo-ku, A. FUJIMORI, U. of Tokyo, Kashiwi, Z. HUSSAIN, Advanced Light Source, Berkeley, Z.-X. SHEN, Stanford U. — Angle resolved photoemission studies in LSCO have revealed a remarkable state of affairs in that the observed Fermi surface maps are in excellent accord with the LDA calculations even in the highly underdoped regime. Here we demonstrate that the agreement with gross band dispersion persists to quite high energy scales of several hundred meV's. For example, even in the 3%-doped sample, the position and shape of the van Hove singularity is found to be in accord with LDA predictions. Signatures of strong correlation physics are manifest however through the suppression of spectral weight near the Fermi energy particularly in the underdoped system. In this way, even though the gross dispersion is virtually unrenormalized, there is a strong renormalization of the spectral weight. Work supported in part by the USDOE.

10:12AM N9.00012 Universal spectral weight transfer in high temperature superconductors, JEFF GRAF, Lawrence Berkeley Lab, GEY-HONG GWEON, KYLE MCELROY, SHUYUN ZHOU, CHRIS JOZWIAK, University of California Berkeley, ELI ROTENBERG, Lawrence Berkeley National Laboratory, Berkeley, ANDREAS BILL, University of California Berkeley, T. SASAGAWA, University of Tokyo, H. EISAKI, AIST, S. UCHIDA, University of Tokyo, H. TAKAGI, DUNG-HAI LEE, ALESSANDRA LANZARA, University of California Berkeley — High resolution angle resolved photoemission spectroscopy (ARPES) studies of the electronic structure of several cuprate families, over the entire phase diagram, from undoped to highly overdoped regime were presented. Evidence of the one-dimensional character of the electronic structure and its evolution with doping will be presented. Similarities and differences of the electronic structure of the nickelates with the stripe phase of other correlated materials as high temperature superconductors and colossal magneto resistance manganesites will be discussed.

10:24AM N9.00013 Spectral properties of the Hubbard-Holstein model and comparison to ARPES experiments in the copper oxides, BRIAN MORITZ, University of Waterloo, ALEXANDRU MACRIDIN, EHSAN KHATAMI, University of Cincinnati, FRANCOIS VERNAY, University of Waterloo, THOMAS MAIER, Oak Ridge National Laboratory, Thomas P. DEVORE, University of Waterloo, MARK JARRELL, University of Cincinnati — We employ a dynamical cluster Quantum Monte Carlo technique to study the two-dimensional Hubbard-Holstein model over a range of fillings, electron-phonon interaction strengths, and phonon frequencies. Previous investigations of the two-dimensional Hubbard model using these techniques have revealed many of the same features as the cuprate superconductors including strong antiferromagnetic correlations and \( d-wave \) superconductivity. We have modified the QMC algorithm to treat a continuous phonon field and take advantage of the long time scales associated with the phonon dynamics to offset the computational expense associated with sampling the relatively large configuration space. The Maximum Entropy method is employed to calculate the real frequency spectrum which we compare and contrast with recent angle-resolved photoemission (ARPES) experiments. We discuss qualitative and quantitative results in the context of features that seem to be universal to the copper oxides.

10:36AM N9.00014 Intermediate Phase in the Superconducting Cuprates,1 TAKESHI EGAMI, University of Tennessee — It has long been speculated that upon doping the Mott-Hubbard insulator may go through an intermediate phase before becoming a Fermi-liquid metal. If there is such a phase its structure may be intimately connected to the mechanism of the pseudogap and superconductivity. The only well-defined and popular option has been the spin-charge stripe phase, but the strongly one-dimensional nature of the stripe phase is at odds with the highly two-dimensional metal. If there is such a phase its structure may be intimately connected to the mechanism of the pseudogap and superconductivity. In this phase the Mott-Hubbard states and the Fermi-liquid phase coexist in different Brillouin sub-zones. The presence of such a phase is consistent with the recent results of the ARPES at a high energy scale (J. Graf, et al., cond-mat/0607319), dispersion of Cu-N bond-stretching phonon mode in YBCO, pulsed neutron PDF analysis of LSCO, and our recent observation of the superlattice peaks in \( \text{YBa}_2\text{Cu}_3\text{O}_6 \) single crystal by x-ray diffraction. The intensity of the superlattice peaks in \( \text{YBa}_2\text{Cu}_3\text{O}_6 \) decreases below 250K. This is an unusual behavior for the ordering peak, suggesting the interplay with superconductivity.

1 Supported by the NSF DMR04-04781

10:48AM N9.00015 Dual character of the electronic structure in \( \text{YBa}_2\text{Cu}_4\text{O}_8 \): conduction bands of \( \text{CuO}_2 \) planes and \( \text{Cu}^0 \) chains, A. KAMINSKI, T. KONDO, R. KHASANOV, J. KARPINSKI, S.M. KAZAKOV, N.D. ZHIGADLO, T. OHTA, H.M. FRETWELL, A.D. PALCZEWSKI, J.D. KOLL, J. MESOT, E. ROTENBERG, H. KELLER, Ames Lab. and Dept. of Physics and Astronomy, Iowa State University — We use a diffraction method to investigate the electronic properties of CuO planes and CuO chains in the high temperature superconductor, \( \text{YBa}_2\text{Cu}_3\text{O}_8 \). In the CuO planes, a two dimensional (2D) electronic structure with nearly momentum independent bilayer splitting is observed. The splitting energy is 150 meV at \( (\pi,0) \), almost 50% larger than in \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) and the electron scattering at the Fermi level in the bonding band is about 1.5 times stronger than in the antibonding band. The CuO chains have a quasi one dimensional (1D) electronic structure. We observe two 1D bands separated by \( \sim 550\text{meV} \): a conducting band and an insulating band with an energy gap of \( \sim 240\text{meV} \). We find that the conduction electrons are well confined within the planes and chains with a non-trivial hybridization.
8:00AM N10.00001 Infrared study of the metal-insulator transition regime in vanadium dioxide^{1}, M. M. QAZILBASH, Physics Department, University of California - San Diego, B. G. CHAE, H. T. KIM, IT Convergence and Components Lab, ETRI, Daejeon, Korea, D. N. BASOV, Physics Department, University of California - San Diego — Vanadium dioxide (VO_{2}) undergoes a metal-insulator transition at T_{I} ≈ 340 K. The transition region of a VO_{2} film has been studied with infrared ellipsometry and near-normal incidence reflectance between 40 cm\(^{-1}\) and 5000 cm\(^{-1}\). The measured optical constants are compared to calculations based on effective medium theories. The anomalies in the frequency and temperature dependence of the optical constants will be presented. The implications of the data for the mechanism of the metal-insulator transition will be discussed.

^{1} This work has been supported by US Department of Energy and ETRI.

8:12AM N10.00002 Metal-Insulator Transition in Ca_{1−x}Na_{x}IrO_{3} with Post-Perovskite Structure, KENYA OHGUSHI, HIROTADA GOTOU, TAKEHIKO YAGI, YOKO KIUCHI, FUMIKO SAKAI, YUTAKA UEDA, Institute for Solid State Physics, University of Tokyo — We developed a novel solid solution Ca_{1−x}Na_{x}IrO_{3} (0 < x < 0.37) with the post-perovskite structure [1, 2]. Upon carrier doping into the S=1/2 antiferromagnetic Mott insulator CaIrO_{3}, the magnetic long-range order is gradually destabilized, culminating in a paramagnetic state at x > 0.30, with simultaneous change from the insulating to metallic behavior. The temperature dependence of the resistivity for metallic samples exhibits several characteristic features: (1) the T\(^{-}\) dependence with α ∼ 1.2 in the metallic range, (2) the lnT\(^{-}\) dependence in the weak-localization regime, and (3) the positive magnetoresistance violating the Kohler’s rule. These results indicate the anomalous metallic state caused by the strong electron correlation effect is realized on the verge of the Mott transition. [1] Nobuyoshi Miyajima, Kenya Ohgushi, Masaki Ichihara, and Takehiko Yagi, Geophys. Res. Lett. 33, L12302 (2006). [2] K. Ohgushi, H. Goto, T. Yagi, Y. Kiuchi, F. Sakai, and Y. Ueda, submitted.

8:24AM N10.00003 Metal-insulating phase transition in YBa_{2}Cu_{3}O_{6+x} by First-Principles, ALESSIO FILIPPETTI — The basic chemistry of YBa_{2}Cu_{3}O_{6+x} represents an historical challenge for first-principles approaches, due to the well known difficulty of standard local-spin density functional theories (such as LSDA or GGA) in describing the correct spin-polarized S=1/2 ground-state of Cu (II) ion. Here we employ the pseudo-SIC approach, which is based on an approximate form of self-interaction corrected (SIC) Kohn-Sham Equations and works well in both Mott-insulating (i.e. x=0) and metallic limit (x=1), to describe the effect of oxygen-doping on the electronic properties of YBa_{2}Cu_{3}O_{6+x}. Our results give a sound description of the order-disorder as well as magnetic-non magnetic phase competitions. We show that the phase transition from the antiferromagnetic insulating to the paramagnetic metal is mainly governed by the ordering of doping oxygens in Cu(I)-O-Cu(I) chains, which in turn, subtly affects the chemistry of Cu(II)-O planes through a non trivial pattern of p-d couplings.

8:36AM N10.00004 Quantum Monte Carlo Study of an Interaction-Driven Band Insulator to Metal Transition^{1}, NORMAN PARIS, University of California, Davis, KARIM BOUADIM, FREDERIC HEBERT, GEORGE BATROUNI, Institut Non-Linear de Nice, UMR 6618 CNRS, Université de Nice-Sophia Antipolis, RICHARD SCALETTAR, University of California — We study the transitions from band insulator to metal to Mott insulator in the ionic Hubbard model on a two dimensional square lattice using determinant Quantum Monte Carlo. Evaluation of the temperature dependence of the conductivity demonstrates that the metallic region extends for a finite range of interaction values. The transitions from band insulator to metal to Mott insulator in the ionic Hubbard model on a two dimensional square lattice using determinant Quantum Monte Carlo. Evaluation of the temperature dependence of the conductivity demonstrates that the metallic region extends for a finite range of interaction values. The Mott phase at strong coupling is accompanied by antiferromagnetic (AF) order. Inclusion of these intersite correlations changes the phase diagram qualitatively compared to dynamical mean field theory.

^{1} NSF DMR 0312261

8:48AM N10.00005 Metal to Nonmagnetic-Insulator Transition in LiVS_{2}, NAOYUKI KATAYAMA, MINORU NOHARA, University of Tokyo, MASAYA UCHIDA, NIMS, HIDENORI TAKAGI, University of Tokyo — LiVS\(_{2}\) has been reported to exhibit a first order magnetic transition with a drastic decrease in susceptibility at about 310 K\(^{[1]}\). In order to clarify the nature of this transition, we performed resistivity, magnetic susceptibility, and electron diffraction measurement for LiVS\(_{2}\). The resistivity in LiVS\(_{2}\) revealed a metal to insular (MI) transition at T_{c} ≈ 310 K. In the insulating state below T_{c}, we observed $\sqrt{3}$a_{B} x $\sqrt{3}$a_{B} superstructure in the electron diffraction, indicating a formation of vanadium trimers in the ab plane. Together with the drastic decrease in susceptibility at T_{c}, we propose a formation of trimer singlet state below T_{c} for LiVS\(_{2}\). Although this ground state is analogous to that observed in the isostructural and isoelectronic oxide LiVO\(_{2}\)\(^{[2]}\), the MI transition is unique to LiVS\(_{2}\). [1] D. W. Murphy et al.; Inorg. Chem. 15 (1976) 17. [2] W. Tian et al.; Mater. Res. Bull. 39 (2004) 1319.

9:00AM N10.00006 Use of Abrikosov-Gorkov Density of States to Extract Spin Polarization at the Metal-Insulator Transition, R. V. A. SRIVASTAVA, W. TEIZER, Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA — We have discovered and applied an analytical solution of the Abrikosov-Gorkov \(^{1}\) density of states (DOS), describing superconductors with impurities, to extract the spin-polarization of 3-dimensional amorphous (a-) Gd_{3}Si_{1−x} in the quantum critical regime (QCR) of a magnetic field tunable metal-insulator transition (MIT). The analysis of the experimental spin-polarized (SP) tunneling conductance of an Al/Al_{2}O_{3}/a-Gd_{3}Si_{1−x} planar tunnel junction at T=25mK in parallel magnetic field H≤3.0T indicates a larger polarization near the MIT of a-Gd_{3}Si_{1−x} (x=0.14) as compared to previous work \(^{2}\), where a SP Bardeen-Cooper-Schrieffer DOS \(^{3}\) was used. We will present polarization values at different applied magnetic fields in the QCR.


9:12AM N10.00007 X-ray absorption spectroscopy studies of Vanadium dioxide thin films across the metal-insulator phase transition boundary. DMITRY RUZMETOV, SHIRIRAM RAMANATHAN, DEAS, Harvard University, Cambridge, MA; SANJAYA D. SENANAYAKE, CSD, Oak Ridge National Lab, Oak Ridge, TN — X-ray absorption (XAS) and photoemission (XPS) spectroscopy of the V 2p edges and O 1s edge was performed on VO₂ thin films synthesized by RF sputtering at various conditions. Distinct changes of the electronic structure depending on the film quality, whether the sample is above or below the metal insulator transition (MIT) temperature, and thermal history of the sample are observed. The spacing between 3dₓ and 3dᵧ band peaks probed by O-edge XAS decreases by 0.8eV with concurrent peak broadening for the sample sputtered at lower substrate temperature and consequently having more polycrystalline and disordered character. There is a similar tendency in the V 2p₁/₂ and 2p₃/₂ edges, i.e. the convergence of the doublets for the disordered sample. The temperature dependence of the XAS V and O edges including repeated crossing of the MIT has been studied. The reversible switches of the 3dₓ and 3dᵧ band peak widths in the O-edge on different sides of the MIT are measured while the peak separation remains the same. The abruptness of the band structure transformation at MIT suggests that the band width changes are determined by the VO₂ MIT phase rather than gradual evolution with temperature.

9:24AM N10.00008 Mott-Hubbard Scenario for the Metal-Insulator Transition in the Two Dimensional Electron Gas . PING SUN, Rutgers University — We exam the experimental observations of the metal-insulator transition in Si-MOSFET and GaAs quantum well. We find that the observed critical behaviors in the magneto transport experiments can be understood within the Mott-Hubbard scenario. Disorder, while playing an important role in both metallic and insulating phases, does not affect the universal critical behaviors.

9:36AM N10.00009 Ni⁢Ⅲ ground state modification through the metal-insulator transition in R⁢N⁢I⁢O₃ perovskites. CINTHIA PIAMONTEZE, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, ALINE RAMOS, HELIO TOLENTINO, Laboratoire de Cristallographie CNRS — R₃NiO₃ perovskites (R=rare earth or Y) present a metal-insulator transition (MIT) with decreasing temperature. For smaller R ions the MIT is explained by a charge ordered state of two nonequivalent Ni sites established in the insulating phase. For the larger R ions the only structural modification observed by diffraction is restricted to a small volume expansion and modifications in the Ni-O-Ni angle. A charge ordered phase for these systems seems to be observed in NdNiO₃ thin films. We have studied systems with R=Pr, Nd and Eu, (MIT temperature 130, 200 and 460K) using X-ray absorption spectroscopy (XAS) at the Ni L-edge. This technique is able to probe the density of unoccupied Ni 3d states, being sensitive to the electronic structure of these systems. A striking difference is observed in the absorption spectra through the MIT. Using theoretical simulations we could propose a model for the MIT based on a low-spin to mixed-spin state transition for Ni³⁺. A very careful measurement of the spectra temperature dependence through the MIT shows a hysteretic behavior as observed in resistivity measurements pointing to the direct correlation between the XAS measurements and the MIT.

2Financial Support: FAPESP, CNPq and DOE

9:48AM N10.00010 2D Wigner crystal: metal to insulator transition via self doping. SERGEY PANKOV, VLADIMIR DOBROSAVLJEVIC, NHMFL-FSU — We consider a scenario of metal to insulator transition in the 2D Wigner crystal. The Wigner crystal is modeled as a two band (bands represent the site and interstitial orbitals) Hubbard model. It is found that the transition is unstable to the electron self doping, resembling conceptually the liquid-solid transition in Helium III. The self doping is shown to stabilize the metallic phase, pushing the transition to lower electron densities. The implication of the self doping to the compressibility, phase separation and transport properties of the Wigner crystal is discussed.

10:00AM N10.00011 Disappearance of the metal-like behavior in GaAs two-dimensional holes below 30mK. JIAN HUANG, Princeton University, JIAN-SHENG XIA, University of Florida, D. C. TSUI, Princeton University, L.N. PFEIFFER, K.W. WEST, Bell Labs, Lucent Technologies — The T-dependence of the resistivity of two-dimensional holes are observed to exhibit two qualitatively different characteristics for a fixed carrier density at temperatures below 100K. In this putatively metallic regime of so-called metal-insulator transition, the sign of the derivative of the resistivity with respect to temperature changes from being positive (dρ/dT>0) to negative (dρ/dT<0) when the temperature is lowered below 30 mK and the resistivity continuously rises with cooling down to 1mK, suggesting a crossover from being metal-like to insulator-like.

1Disappearance of the metal-like behavior in GaAs two-dimensional holes in GaAs below 30mK

10:12AM N10.00012 Metal-insulator transition and domains in suspended VO₂ nanobeams. JIANG WEI, WEI CHEN, ZENGHUI WANG, DAVID COBDEN, University of Washington — VO₂ undergoes a metal-insulator transition (MIT) around 67°C. We investigate the transition in suspended crystalline nanobeams of VO₂. The nanobeams are grown by vapor phase deposition on SiO₂ substrates and contacted by electron beam lithography with chromium-gold metallisation. After suspended them by selectively etching away the substrate, the resulting nanobeams are firmly clamped at the contacts. Under some conditions the MIT occurs suddenly throughout the entire beam, associated with a single hysteretic conductance jump. This is in contrast with the behavior of nanobeams attached to the substrate in which alternating metallic and insulating domains form during the transition. Under other conditions, a single metallic domain forms and grows gradually as temperature is increased. At room temperature the longer beams are buckled, and on warming they unbuckle when the MIT occurs. When a force is applied to bend a suspended nanobeam, alternating domain patterns form in the bent region reflecting the strain field.

2Work supported by US Army Research Office

10:24AM N10.00013 Physical properties of VO₂ and V₂O₅ nanowires. WEI CHEN, JIANG WEI, DAVID COBDEN, University of Washington — Both VO₂ and V₂O₅ show dramatic metal-insulator transitions, whose manifestations on the nanoscale are not known. We investigate techniques to differentiate and pattern the metallic and insulating domains in small VO₂ crystals and nanowires grown by vapor phase deposition. For instance, it has been reported that insulating VO₂ can be metallized by electron beam exposure and by hydrogenation. We attempt to distinguish the domains by scanning probe techniques, including topography and electric force microscopy, and observe a pinning effect of the domains by oscillating strain variations when the nanowire is attached to a substrate. When the strain is released by etching, the pinning is removed. The VO₂ crystals can be converted to V₂O₅ crystals by reducing in hydrogen and annealing. By patterning the V₂O₅ on the nanoscale we aim to realize strongly correlated quantum dots.

3Work supported by US Army Research Office

10:36AM N10.00014 Orientation Studies of Recrystallized Vanadium Dioxide . FELIPE RIVERA, MIKE CLEMEMS, Brigham Young University, LAUREL BURK, University of Nebraska - Lincoln, ROBERT DAVIS, RICHARD VANFLEET, Brigham Young University — Crystalline films and isolated vanadium dioxide particles were obtained through thermal annealing of amorphous vanadium dioxide thin films on silicon dioxide. Vanadium dioxide undergoes an insulator to metal transition near 66 °C. Orientation Imaging Microscopy (OIM) was used to study the phase and orientation of the crystals formed, as well as to differentiate from different vanadium oxide crystal structures. Kikuchi patterns for the tetragonal phase of vanadium dioxide were used for indexing as the Kikuchi patterns for the two phases are indistinguishable by OIM. There is a preferred orientation for the growth of these crystals with the c axis of the tetragonal phase parallel to the plane of the specimen. Resistance and Capacitance measurements on these films are being performed to study the electronic characteristics of this phase transition. The results of this study will be presented.
The optical conductivity of Ni originates in electron promotion, localization, and defect induced quasiparticle formation.

Using small polaron fits we individualize these as related to glass stretching vibrational modes. The electron scattering rate denotes an unique relaxation time characteristic of a single type of carriers and has a very strong temperature dependence due to strong electron-phonon interactions. Using small polaron fits we individualize these as related to glass stretching vibrational modes. The electron scattering rate denotes an unique relaxation time characteristic of a single type of carriers and has a very strong temperature dependence due to strong electron-phonon interactions.

The higher Curie temperatures are regarded as one of the promising materials of room-temperature ferromagnetism because its intrinsic nature was confirmed through magnetic circular dichroism (MCD) measurement[2]. In this presentation, we report the effect of co-doping of charge impurities on ferromagnetic properties in this material. It was found that ferromagnetism was suppressed in (Zn,Co)Te co-doped with nitrogen (N) as an acceptor impurity[3] and was enhanced in a crystal co-doped with iodine (I) as a donor impurity[4]. In particular, the apparent Curie temperature $T_C$ of Zn$_{1-x}$Co$_x$Te with a Co concentration of $x = 0.05$ increased up to 300K at maximum due to I-doping, compared to $T_C \sim 300K$ in the undoped crystal. In the structural and compositional analysis using TEM/EDS, it was revealed that the origin of this remarkable effect of the co-doping was the variation of Cr distribution in the crystals; the Cr distribution was strongly inhomogeneous in I-doped crystals with higher $T_C$, in contrast to an almost uniform distribution in undoped or N-doped crystals with lower $T_C$ or being paramagnetic. In the crystals of inhomogeneous distribution, Cr-rich regions with a typical size of several ten nanometers formed in the Cr-poor matrix act as ferromagnetic nanoclusters, resulting in an apparent ferromagnetic behavior of the whole crystal. These variation of the Cr uniformity can be linked to a change in the Cr charge state due to the co-doping, which is considered to affect the aggregation energy of Cr ions in the host compound ZnTe[5]. These findings will open a new way to control the formation of magnetic nanoclusters in the semiconductor matrix and ferromagnetic properties by manipulating the charge state of magnetic impurities.

We reveal that


1 Supported by US ONR and NSF-ECCS Career.
We consider ferromagnetism in spatially randomly located magnetic moments, as in a diluted magnetic semiconductor, coupled via the carrier-mediated indirect exchange RKKY interaction. We obtain, via Monte Carlo calculations, the magnetic phase diagram as a function of the impurity moment density \( n_i \) and the relative carrier concentration \( n_c/n_i \). As evidenced by the diverging ferromagnetic correlation length and magnetic susceptibility, the boundary between ferromagnetic and nonferromagnetic phases constitutes a line of zero temperature critical points which can be viewed as a magnetic percolation transition. In the dilute limit, we find that bulk ferromagnetism vanishes for \( n_c/n_i > 0.1 \). We also incorporate the local antiferromagnetic direct superexchange interaction between nearest neighbor impurities and examine the impact of a damping factor in the RKKY range function. This work has been done in collaboration with Sankar Das Sarma at the University of Maryland and supported by the US-ONR and NSF.

We present numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state.

We present numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state.

We present numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state.

We present numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state.

We present numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state.

We present numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state.

We present numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state. We find numerical results of the nature of single particle states in such a positionally disordered three-dimensional system with a maximally self-averaging ground state.
10:48AM N12.00011 Complexities in diluted magnetic semiconductors-a theoretical perspective from ab-initio electronic structure calculations, BIPLAB SANYAL, DIANA IUSAN, OLLE ERIKSSON, Department of Physics, Uppsala University, Sweden — Diluted magnetic semiconductors (DMS), the essential materials for semiconductor spintrons, show a variety of complex properties, e.g., defect-mediated (ferro/antiferro)magnetic interactions and the disorder leading to magnetic percolation effects. Using the ab-initio Korringa-Kohn-Rostoker-Coherent-Potential-Approximation, the magnetic pair exchange parameters of a Heisenberg model have been calculated for Mn doped ZnO and half-Heusler NiTiSn hosts followed by the calculation of transition temperatures using Monte-Carlo simulations. Zinc vacancies and nitrogen substituting oxygen atoms lead to ferromagnetic interactions in Mn doped ZNO while in a defect free case, the interaction between Mn atoms is antiferromagnetic. The calculated critical temperatures are low (~35 K) due to the short-range exchanged interactions and low defect concentration. In the other case, Mn doped NiTiSn shows a high critical temperature (~300 K) for 22 % Mn concentration. Below 3% Mn, there is no magnetic long range order as the magnetic percolation is not established. The results are in good agreement with experiments.

Wednesday, March 7, 2007 8:00AM - 11:00AM —
Session N13 DMP GMAG: Focus Session: Multiferroics IV Colorado Convention Center Korbel 4C

8:00AM N13.00001 Multiferroic Domain Dynamics and Phase Transitions in Strained SrTiO$_3$ Films, S. DENEV, A. VASUVADERAO, A. KUMAR, M. BIEGALSKI, Y. LI, L-Q. CHEN, S. TROLIER-MCKINSTRY, D. SCHLOM, V. GOPALAN, Dept. of Materials Science and Engineering, Pennsylvania State University — SrTiO$_3$ is a material that is not normally ferroelectric or multiferroic at any temperature. However, epitaxial biaxial strain in thin film form can induce multiferroicity in strained SrTiO$_3$ (J.H.Haeni et al., Nature 430,758 (2004)). We have demonstrated multiferroicity in strained SrTiO$_3$ films on scandate substrates, with the presence of two independent order parameters, a polar ferroelectric polarization vector, and an axial antiferrodistortive rotation vector. Using Optical Second Harmonic Generation (SHG), we have distinguished these axial and polar properties, tracked the ferroelectric and antiferrodistortive phase transitions as a function of temperature, and determined the point group symmetry of the ferroelectric and multiferroic phases. For the first time, we have shown direct imaging of ferroelectric domains and revealed the mechanism of coupled switching of ferroelectric-ferroelastic domains under electric fields using piezolectric force microscopy combined with phase field simulations. (Phys. Rev. Lett., Accepted, in print (2006)). These studies have broader relevance to multiferroics with coupled polar and axial order parameters, such as ferroelectric antiferromagnets.

8:12AM N13.00002 Broadband IR Spectroscopy of Multiferroic BiFeO$_3$, J. SEIDEL, C.L.S. KANTNER, Y.-H. CHU, L. YANG, Z. SCHLESINGER, D. VIEHLAND, J. ORENSTEIN, R. RAMESH, University of California, Berkeley — BiFeO$_3$ (BFO) is a multiferroic material in which both the ferroelectric and antiferromagnetic ordering is present at room temperature. In order to investigate the dynamics of the coupling between order parameters, optical spectroscopy measurements were made on both a single crystal and epitaxially grown thin film samples. Measurements were made from 3-30cm$^{-1}$ using time domain terahertz spectroscopy, and from 20-700 cm$^{-1}$ with FTIR reflectivity. We report on the spectral weight and damping of modes in BFO in the spectral region where antiferromagnetic resonance is typically observed in orthoferrites.

8:24AM N13.00003 Electrodynamics of a multiferroic perovskite manganite in terahertz frequency range$^{1}$, N. KIDA, ERATO-JST, Y. IKEBE, R. SHIMANO, Y. YAMASAKI, Univ. Tokyo, T. ARIMA, ERATO-JST and Tohoku Univ., Y. TOKURA, ERATO-JST, CERC-AIST, and Univ. Tokyo — There is a growing interest for the study of the magnetoelectric effect, as stimulated by the observation of a magnetic control of the ferroelectric polarization in perovskite manganites. Recently, a broad peak structure was observed in TbMnO$_3$ and GdMnO$_3$ in terahertz (THz) frequency range$^{1}$. The spin-wave excitation driven by ac electric field, which is referred to as electromagnon, was proposed as an origin of this structure. However, detailed characteristics, especially, the role of the rare-earth ion and the relationship between the complex dielectric constant $\varepsilon$ in THz and low ($\sim$kHz) frequency range were not clarified yet. Here we used the THz time-domain spectroscopy to directly extract $\varepsilon(\omega)$ (1.2–4.5 meV) of a multiferroic perovskite manganite and discuss the origin of the ferroelectricity, as manifested by a gigantic response of the low-frequency $\varepsilon(\omega)$ with temperature and magnetic fields. $^{1}$A. Pimenov et al., Nat. Phys. 2, 97 (2006).

$^1$This work was in part supported by a Grant-In-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan.

8:36AM N13.00004 Magnetolectric Emission in a Magnetic Ferroelectric Er-doped (Ba,Sr)TiO$_3$, YOSHI-AKI SHIMADA, Department of Applied Physics, University of Tokyo, MASAKAZU MATSUBARA, Correlated Electron Research Center, National Institute of Advanced Industrial Science and Technology, YOSHIO KANEKO, JING-PING HE, Spin Superstructure Project, ERATO, Japan Science and Technology Corporation, YOSHINORI TOKURA$^1$, Department of Applied Physics, University of Tokyo — In the system where both space-inversion ($I$) and time-reversal ($\mathcal{R}$) symmetries are broken simultaneously, a nonreciprocal optical phenomenon termed the optical magnetoelectric (OME) effect is expected to show up. As the crystal that has neither $I$ nor $\mathcal{R}$ symmetry, we have investigated an Er$^{3+}$-doped ferroelectric (Ba,Sr)TiO$_3$ single crystal under magnetic field in which the luminescent magnetic Er$^{3+}$ ion occupies a noncentrosymmetric site. The $k$-directional dichroism derived from the OME effect was verified in the $2.5\mu$m emission by the reversal of magnetic field and spontaneous polarization. The observed nonreciprocity $\Delta I/\sim 0.5 \%$ at 3000 Oe implies the possibility of the application of the OME effect to the function of an optical isolator.

$^1$Also at Correlated Electron Research Center, National Institute of Advanced Industrial Science and Technology, Spin Superstructure Project & Multiferroics Project, ERATO, Japan Science and Technology Corporation.

8:48AM N13.00005 Colossal magnon-phonon coupling in multiferroic Eu$_{0.75}$Y$_{0.25}$MnO$_3$, ROLANDO VALDES AGUILAR, A.B. SUSHKOV, H.D. DREW, MRSEC, University of Maryland, College Park, MD 20742, C. ZHANG, S.-W. CHEONG, Rutgers University, Piscataway, NJ 08854 — The temperature dependence of the far infrared (IR) transmission spectra (1-30 meV) of multiferroic Eu$_{0.75}$Y$_{0.25}$MnO$_3$ has been measured. This system is chosen to correspond to TbMnO$_3$ but without the magnetism of the rare earth ion. We find a spectacular transfer of spectral weight from the lowest frequency IR active phonon to a magnetic excitation, at lower frequencies, when light is polarized parallel to the static polarization $P_s$. We also observe the electromagnon at a frequency of 2.5 meV, with the same selection rule. The electromagnon produces the observed increase in the dielectric constant as the system enters the ferroelectric phase. The observations of large spectral weight transfer and of the electromagnon selection rule, are not consistent with the model of the electrically response of helical magnets proposed by Katsura, et al.$^3$$^3$ We compare and contrast these results to other multiferroic manganites.

9:00AM N13.00006 Giant magnetoelastic effect in multiferroic Ba$_0.4$Sr$_1.4$Zn$_2$Fe$_{12}$O$_{22}$. DIYAR TAL-BAYEV, RICHARD D. AVERITT, ANTOINETTE J. TAYLOR, Los Alamos National Laboratory, TSUYOSHI KIMURA, Bell Laboratories — Dynamical studies of multiferroic materials help unravel the fundamental interactions between various degrees of freedom and answer technological questions such as achievable switching speeds in multiferroic-based memory elements. We report the results of the ultrafast optical study of multiferroic Ba$_0.4$Sr$_1.4$Zn$_2$Fe$_{12}$O$_{22}$, which reveals a giant magnetoelastic effect in the material. The compound exhibits a hexagonal crystal structure and a helical magnetic ground state below $\sim 330$ K. In applied magnetic field, the hexaferrite undergoes a series of magnetic phase transitions and develops ferroelectric polarization. The magnetoelastic effect is detected via the evolution of the speed of sound in the crystal as a function of magnetic field. The oscillation in the optically induced transient reflectivity resulting from the propagating coherent-phonon strain pulse allows us to measure the field-induced changes in the speed of sound and the corresponding dramatic changes in the elastic stiffness. The dependence of the exchange interaction on the distance between Fe ions gives rise to the observed magnetoelasticity. Our results indicate a route towards the magnetically modulated transducers and piezoelectric devices.

9:12AM N13.00007 Far-infrared transmission spectroscopy studies of HoMn$_2$O$_5$ single crystals at the commensurate-incommensurate phase transition. A. A. SIRENKO, Department of Physics, New Jersey Institute of Technology, Newark, NJ 07102, S. PARK, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, S. M. O’MALLEY, Department of Physics, New Jersey Institute of Technology, Newark, NJ 07102, G. L. CARR, NSLS, Brookhaven National Laboratory, Upton, New York 11973, S.-W. CHEONG, Rutgers Center for Emergent Materials, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854 — Spectra of the low-frequency IR-active excitations in HoMn$_2$O$_5$ multiferroic single crystals have been studied using synchrotron radiation based far-infrared transmission spectroscopy at U12R beamline of NSLS-BNL in the frequency range between 8.5 and 105 cm$^{-1}$. Both preferable polarization of IR-active excitations along crystallographic directions of HoMn$_2$O$_5$ and temperature variation of their oscillator strength reveal strong changes at the commensurate-incommensurate phase transition at $T_{\text{J}} = 19$ K. Transmission spectra are interpreted in terms of the electromagnon, magnon, and crystal-field splitting excitations.

9:24AM N13.00008 Electromagnons in multiferroic RMn$_2$O$_5$ compounds. ANDREI SUSHKOV, ROLANDO VALDES AGUILAR, DENNIS DREW, University of Maryland, SOONYONG PARK, SANG-WOOK CHEONG, Rutgers University — Electromagnons, or magnons with electric dipole activity, were observed so far only in some multiferroic RMnO$_5$ and RMn$_2$O$_5$ compounds. Electromagnons in these two systems have essentially different properties. We try to take a systematic look at electromagnons in the whole RMn$_2$O$_5$ family. In this talk, we report the results of detailed infrared study$^1$ of YMn$_2$O$_5$ and TbMn$_2$O$_5$ as well as some results on other RMn$_2$O$_5$ compounds. We found that electromagnons in the RMn$_2$O$_5$ family is a property of the manganese sublattices. The electromagnon spectrum consists of a set of well defined far infrared ($3\text{−}80$ cm$^{-1}$) modes which are just slightly broader than uncoupled magnons. No obvious changes in the phonon spectrum have been observed. Polarization of electromagnons is in agreement with the dominating symmetric exchange. $^*$ A. B. Sushkov, R. Valdes Aguilar, S. Park, S-W. Cheong, and H. D. Drew, cond-mat/0608707.

9:36AM N13.00009 Magnons and electromagnons in multiferroic materials. MAXIM MOSTOVOY, Materials Science Center, University of Groningen — The interest in studying excitations in frustrated magnets lies in their unusual nature and strong effect on frustrated ordering. The coupled spin-lattice dynamics in frustrated magnets, in which magnetic ordering breaks inversion symmetry and induces electric polarization, was recently studied in optical absorption and neutron scattering experiments. I will present a theory of magnetic excitations coupled to polar phonon modes (electromagnons) in multiferroic materials showing incommensurate magnetic orders, e.g. RMnO$_5$, Ni$_2$V$_2$O$_7$, and MnWO$_4$, and discuss the evolution of the excitation spectrum at the transition from the paraelectric sinusoidal to the ferroelectric spiral state. The incommensurate orders give rise to a multi-band structure of magnetic excitations, while the magnetoelectric coupling makes possible to excite magnons by oscillating electric field. Even for weak driving the probability of electro-excitation of magnons is relatively large. Furthermore, the polarization dependence of the optical absorption makes possible to discriminate between the electromagnon and antiferromagnetic resonance peaks. I will also discuss electromagnons in a different class of multiferroics, such as the RMn$_2$O$_5$ compounds.

9:48AM N13.00010 Theory of electrical control of spin waves in multiferroic materials. ROGERIO DE SOUSA, JOEL MOORE, University of California, Berkeley — We consider the question of electrical generation, control, and detection of magnons in thin films of multiferroic BiFeO$_3$. This material possesses simultaneous ferroelectric and antiferromagnetic order, with Dzyaloshinskii-Moriya and other magnetoelectric couplings. The spectrum for the coupled spin and polarization waves is found to be extremely anisotropic, allowing the control of spin waves via electrical switching of the direction of the spontaneous polarization vector. Electrical generation and detection of spin waves is optimal at the anticrossings of the polarization and magnetic branches, where the excitations have electromagnon character.

10:00AM N13.00011 Temperature-dependent Raman spectroscopy of multiferroic TbMn$_2$O$_5$. J. R. SIMPSON, A. R. HIGHT WALKER, National Institute of Standards and Technology, Gaithersburg, MD 20899, R. VALDES AGUILAR, A. B. SUSHKOV, H. D. DREW, University of Maryland, College Park, MD 20742, S. PARK, S.-W. CHEONG, Rutgers University, Piscataway, NJ 08854 — Multiferroic materials that display coupling between order parameters, e.g., magnetic and dielectric, stimulate fundamental interest and provide the potential for applications in novel multifunctional devices. The multiferroic manganese TbMn$_2$O$_5$ exhibits non-collinear magnetic order and a strong magnetoelectric coupling effect. The recent observation$^2$ of infrared (IR) phonon correlated with magnetic and dielectric phase transitions suggests a complementary Raman study may provide important information regarding the nature of coupling in these systems. We present Raman measurements of single-crystal TbMn$_2$O$_5$ in a collinear backscattering configuration as a function of temperature ($4 \text{−} 300$ K) and polarization along various crystallographic axes. Additionally, we compare the temperature dependence of Raman active phonons with the activation of an IR forbidden mode in the low-temperature ferroelectric state.

$^1$This work is supported by NSF (DMR 0546985); NSLS is supported by DOE (DE-AC02-98CH10886)

$^2$This work supported in part by NSF-MRSEC Grant DMR-0520471.

$^3$We acknowledge support from the Western Institute of Nanoelectronics (WIN).

$^4$Work supported, in part, by the NIST-NRC postdoctoral fellowship.

10:12AM N13.00012 Magnetic properties and electronic structure of doped multiferroic Y_{2−x}A_{x}MnO_{3} (A=Ca, Sr, Ba) , J. Y. JUANG, Electrophysics, National Chiao-Tung University, C. C. HSIEH, T. Y. CHENG, J. M. LEE, J. M. CHEN, J.-Y. LIN, K. H. WU, T. M. UEN, Y. S. GOU — We report the magnetic properties, X-ray absorption spectroscopy (XAS) on a series of doped multiferroic materials Y_{2−x}A_{x}MnO_{3} (A=Ca, Sr, Ba). YMnO_{3} when doped by alkaline-earth metal with various ionic sizes, display dramatic changes in magnetic properties as compared with the parent compound. For Ca-doped sample, the antiferromagnetic (AFM) phase transition appears to take place at a much lower temperature (30 K) as compared to that of undoped one (42 K), which could be Mn-rich. On the other hand, when doped with ions of larger size such as Ba and Sr, the AFM temperature decreased only slightly to around 38 K but with significantly smeared transition. By comparing the XAS results to standard manganese oxide powder, YMnO_{3} exhibits the dominant Mn^{3+} characteristics obtained from the standard Mn_{2}O_{3} powder. Although, the undoped-YMnO_{3} and Sr-, Ba-doped YMnO_{3} exhibited very similar electronic structure as revealed in the XAS data, the XAS of Ca-doped sample, again, is very different from that of YMnO_{3}. It is surprising to observe that Ca-doping has resulted in most significant modifications in the magnetic property and electronic structure of YMnO_{3}, since Ca^{2+} is having exactly the same ionic size as that of Y^{3+} and is expected to cause minimal distortion on the lattice.

10:24AM N13.00013 Multiferroic Behavior in Barium Hexaferrite Probed with Optical Second Harmonic Generation , EFTIHIA VLAHOS, SAVA DENEV, VENKATRAMAN GOPALAN, Pennsylvania State University, TSUYOSHI KIMURA, Bell Laboratory, Lucent Technologies, PENNSYLVANIA STATE UNIVERSITY COLLABORATION, BELL LABS COLLABORATION — Barium hexaferrite B_{10.5}Sr_{1.5}Zn_{2}Fe_{12}O_{22} is a very promising material, which exhibits significant magnetoelectric (ME) effect, i.e., the generation of electric polarization/magnetization by the application of magnetic/electric field. Optical second harmonic generation (SHG) in the reflection geometry was used to determine the magnetic point group symmetries and phase transitions of the sample versus temperature, and variable magnetic field. Simultaneous measurements of magnetocapacitance, and ME current as functions of temperature and applied magnetic field are performed and correlated with SHG measurements.

10:36AM N13.00014 Observation of local non-centrosymmetry in weakly ferroelectric YCrO_{3} , ANNA LLOBET, KANNADAKA RAMESHA, THOMAS PROFFEN, Lujan Neutron Scattering Center, Los Alamos National Laboratory, C.R. SERRAO, C.N.R. RAO, Chemistry & Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research — Using high resolution neutron powder diffraction we have determined the average and local structure of YCrO in order to explain the recently reported ferroelectric character YCRO. Unlike other ferroelectric systems, YCRO has been found to have a centrosymmetric crystal structure which is inconsistent with the development of electric polarization because it requires atomic off-centering. We have characterized the different length scales existent in YCRO and found that, although the average crystallographic structure above and below the ferroelectric transition is orthorhombic and centrosymmetric (Pnma), in the ferroelectric state YCRO is locally non-centrosymmetric and Cr is displaced about 0.01 Å from its position along z direction. We conclude that the local character of the Cr off-centering and the small value of the displacement observed could explain the weak ferroelectric behavior. This new concept of “local non-centrosymmetry” might be of great importance for the understanding of unusual properties of other multifunctional materials as well.

10:48AM N13.00015 Computational study of the ferromagnetic and ferroelectric properties of (Bi_{2}Mn NiO_{6})_{4} , LEONARD KLEINMAN, B.R. SAHU, ADRIAN CIUCIVARA, University of Texas at Austin — Using the VASP PAW code with the GGA and including spin-orbit coupling and allowing for non collinear magnetization, we performed electronic structure calculations for the multiferroic crystal, (Bi_{2}Mn NiO_{6})_{4}. The lattice angle and lattice constants are in excellent agreement with experiment. The magnetization is 4.94 \mu B. The polarization, for which there is no experimental value, is 16.84 \mu C/cm^{2}. Inverting the positions of all the atoms we iterated to convergence. The magnetization did not change and the total energy was also unchanged. Thus we conclude that the polarization and magnetization are uncoupled and (Bi_{2}Mn NiO_{6})_{4} is unlikely to have any device applications.

Wednesday, March 7, 2007 8:00AM - 11:00AM — Session N14 GMAG DMP FIAP: Focus Session: Current Induced Magnetization Dynamics and Spin Transfer Colorado Convention Center Korbel 4D

8:00AM N14.00001 Temperature rise due to Joule heating in a spin transfer torque nano-pillar structure1 , CHUN-YEOL YOU, SEUNG-SEOK HA, Dept. of Physics, Inha University, HYUN-WOO LEE, Dept. of Physics, Pohang University of Science and Technology — Considering that the spin-transfer-torque-induced magnetization dynamics in a nano-pillar structure usually requires a large current density of 10^{11} A/m², it is desired to have an accurate estimation of the temperature rise caused by the current-induced Joule heating. We investigate the current-induced heating effect in the nano-pillar by analytical and numerical methods. We employ the Green’s function method to obtain analytic solution of the heat conduction equation. With proper approximations, we derive a simple analytic relation that expresses the temperature in term of the current density, the geometry of the nano-pillar, and material properties. The validity of the analytic expression is confirmed by the comparisons with commercial finite element method software.

1This work was supported by the Korea Research Foundation Grant funded by the Korean Government (MOEHRD) (KRF-2005-070-C00053).

8:12AM N14.00002 Current-Hysteretic Low Frequency Oscillations in Spin-Transfer Nanocontacts , MATTHEW PUFALL, WILLIAM RIPPARD, MICHAEL SCHNEIDER, THOMAS SILVA, STEPHEN RUSSEK, National Institute of Standards and Technology, 325 Broadway, Boulder, CO 80305 — We have observed spin-transfer-driven large amplitude, current hysteretic, low frequency (< 500 MHz) oscillations in nanocontacts made to spin valve structures. The oscillations occur only for small (<50 Oe) in-plane applied fields, but persist in fields up to several kOe for out of plane fields. The frequency of oscillation is typically far below the uniform-mode ferromagnetic resonance frequency, and is only a weak function of applied field. Hysteresis in the presence/absence of the oscillations is observed with dc current, with oscillations first appearing at high currents with increasing current, but persisting to lower currents upon decreasing the current. We suggest that these observations are consistent with dynamics of a vortex-like state in the vicinity of the contact, one nucleated by the Oersted fields generated by the dc current, and with dynamics driven by the spin transfer torque. The electrical oscillation amplitudes are large, with the largest amplitudes approaching 1 mV, and are narrowband, with many devices exhibiting sub-megahertz linewidths.
8:24AM N14.00003 Thermal effects in spin torque switching, MICHAEL SCHNEIDER, MATTHEEW PUFAIL, WILLIAM RIPPARD, STEPHEN RUSSEK, National Institute of Standards and Technology, JORDAN RATINE, Hitachi Global Storage — We compare low temperature device behavior with room temperature behavior. We find agreement between our low temperature critical current measurements and Slonczewski theory1. In addition, we find that the values extrapolated from the low temperature measurements were robust with respect to device size. At room temperature we find substantial variation in the hysteretic region from device to device for devices of the same nominal size. While this is not expected, it has been attributed to thermal effects having a strong influence on the response of the freellayer to applied field as well as the coercivity2. We find that by reducing the temperature, and thus any thermal fluctuations, the device to device variations are drastically reduced. While we did observe indications of non-single domain behavior at 5 K, it is noteworthy that these did not seem to affect the critical switching current. Thus, we conclude that the room temperature device to device variations in the quasi-static switching behavior is dominated by thermal effects. 1. J. C. Slonczewski, J. Magn. Magn. Mater. 159, L1-L7 (1996) 2. D. Lacour, J. A. Katine, N. Smith, M. J. Carey, and J. R. Childress, 85, 4681-4683 (2004).

8:36AM N14.00004 Nonlocal magnetization dynamics, YAROSLAV TSERKOVNYAK, University of California, Los Angeles — Recently, nonlocal properties of ferromagnetic dynamics in magnetic nanostructures, such as damping sensitive to the Ohmic environment and spin-wave transfer between exchange-decoupled ferromagnets, have attracted a considerable interest [1]. It is also becoming clear [2] that nonlocal dynamic effects are important for understanding intrinsic properties such as magnetic damping, noise, and spin-transfer torques in inhomogeneous ferromagnets, with consequences for phenomena ranging from spin-wave propagation and domain-wall motion to current-driven instabilities in the bulk. I will present a self-consistent mean-field approach for treating these properties in a unified and rather general fashion. [1] Y. Tserkovnyak, A. Brataas, G. E. W. Bauer, and B. I. Halperin, Rev. Mod. Phys. 77, 1375 (2005) [2] Y. Tserkovnyak, H. J. Skadsem, A. Brataas, and G. E. W. Bauer, Phys. Rev. B 74, 144405 (2006)

9:12AM N14.00005 Precession damping in itinerant ferromagnets, KEITH GILMORE, MARK STILES, National Institute of Standards and Technology, YIVES IDZERDA, Montana State University — The damping of excited magnetic states has long been understood at a phenomenological level through the Landau-Lifshitz-Gilbert equation. Increased interest in nanoscale devices, the behavior of which can be strongly dependent on the damping, has led to a more theoretical approach. While we consider the simpler 3d transition metals (iron, nickel, and cobalt) in order to understand the most basic processes involved in damping before approaching the more complicated mechanisms expected in alloys. Resistance experiments for Co and Ni indicate low and high temperature regions for which the damping parameter is roughly proportional and inversely proportional, respectively, to the scattering time. We report and numerically test a model that produces both of these behaviors. As with all previous work, the calculations presented are given in terms of an unknown electronic scattering time. To make meaningful comparisons between the calculated and measured damping parameters we evaluate an expression for the conductivity, derived by similar methods, and compare also to transport experiments.

9:24AM N14.00006 Fast Pulse Measurements and Temperature Variation of Enhanced Magnetic Damping of Spin-Transfer Excitation, E. M. RYAN, A. G. F. GARCIA, P. M. BRAGANCA, G. D. FUCHS, N. C. EMLEY, J. C. READ, E. TAN, D. C. RALPH, R. A. BUHRMAN, Cornell University, J. A. KATINE, Hitachi G.S.T. — Recently, light terbium (Tb) doping in thin films of permalloy (Py) has been shown to increase the damping parameter α by several orders of magnitude [1]. To directly study the effect of increased α on spin-transfer systems, we have fabricated 0.004 mm2 Py/Cu/Py nanopillar spin valves with 0 and 2% Tb in the free layer, and measured critical currents across a range of temperatures from 4.2 K to 295 K. We find that the critical currents for reversibly switching the free layer, generally expected to be proportional to α, are several times larger on average in the 2% Tb samples than in pure Py samples, and increase linearly with decreasing temperature. We will also discuss FMR data, and data for switching with fast pulses from 1 to 100 nsec at both 150 K and room temperature, along with matching simulations that allows us to extract α and other spin-torque parameters [2]. These results suggest one approach for controllably reducing the negative impact of spin-torque effects on nanoscale spin valve and read head sensors, and achieving a deeper understanding of these spin-torque devices. [1] W. Bailey, P. Kabos, F. Mancoff, and S. E. Russek, IEEE Trans. Magn. 37, 1749 (2001). [2] P. M. Braganca, et al. Appl. Phys. Lett. 87, 112507 (2005).

9:36AM N14.00007 Modeling study on the self-consistent feedback between inhomogeneous magnetization and the spin torque, KYUNG-JIN LEE, Korea University, BERNARD DIENY, SPINTEC, URA CEA-CNRS, France — The Slonczewski's spin term was originally suggested within the context of homogeneous magnetic domain. Micromagnetic [1] and experimental [2] studies have revealed that the magnetizations excited by the spin torque could be inhomogeneous. Therefore we have to find a way of correcting the Slonczewski's terms in describing the magnetization dynamics. We show the self-consistent model to numerically solve the equations of motion of local magnetization and spin accumulation. The self-consistent model enables us to consider the feedback between inhomogeneous magnetization and the spin torque. We found the feedback is crucial in the magnetization dynamics induced by the spin torque. We will show the computational evidence of the importance of the feedback for the current-induced magnetic excitation in a single Co layer and a spin valve structure. [1] K. J. Lee et al. Nat. Mat. 3, 877 (2004); Appl. Phys. Lett. 88, 132506 (2006), [2] Y. Acremann et al. Phys. Rev. Lett. 96, 217201 (2006).

9:48AM N14.00008 Planar Spin-Transfer Device with a Dynamic Polarizer, YAROSLAV BAZALIY, Institut Loizent, Leiden University, The Netherlands and Dept. of Physics and Astronomy, University of South Carolina, DEBO OLASEBEKAN, Dept. of Physics, Cornell University, BARBARA JONES, IBM Almaden Research Center — In planar nano-magnetic devices magnetization direction is kept close to a given plane by the large easy-plane magnetic anisotropy (e.g. by shape anisotropy in a thin film). In conventional micromagnetics it is known that in this case the magnetization motion is effectively in-plane with only one angle required for its description, and can become overdamped even for small values of the Gilbert damping. We extend the equations of the effective in-plane dynamics to include the spin-transfer torques. The simplifications achieved in the overdamped regime allow us to study systems with several dynamic magnetic pieces (“free layers”). A transition from a spin-transfer device with a static polarizer to a device with two equivalent magnets is observed: when the size difference between the magnets is less than critical, the device does not exhibit switching, but goes directly into the “windmill” precession state.

10:00AM N14.00009 Role of Spin dependent Inelastic Scattering in Spin Torque Devices, SAYEEF SALAHUDDIN, SUPRIOY DATTA, ECE, Purdue University — Spin torque devices are commonly modeled by looking only at the spin dependent transmission and reflection at the tunnel oxide-ferromagnet interface. Here, we describe a different approach where, in addition to barrier dependent phenomena, an inelastic spin-flip scattering is included at the interface. We show that such scattering events may have significant influence on the device behavior, specifically on the magnitude of TMR and on the efficiency of spin torque. We shall show that recent experiments provide evidence for this prediction. Our transport model is based on Non Equilibrium Green’s Function (NEGF) formulation where the scattering is included through a self energy matrix. We also discuss how the spin flip scattering may help to reduce the switching current necessary to flip the magnetization in penta-layer spin torque devices, a phenomenon demonstrated in recent experiments [1].

10:12AM N14.00010 Spin-polarized scanning tunneling microscope and the Kondo effect. KELLY PATTON, STEFAN KETTEMANN, I. Institut fur Theoretische Physik Universitat Hamburg, Hamburg 20355 — We calculate the tunneling current between a spin-polarized scanning tunneling microscope (SP-STM) and a Kondo impurity on a metallic substrate, including the effects of the spin-polarization of the SP-STM on the adsorbate. This spin-polarization breaks the spin symmetry of the Kondo system, similar to an applied magnetic field, which leads to a splitting of the Abrikosov-Suhl-Kondo resonance. The amount of splitting is controlled by the strength of the coupling between the impurity and the SP-STM tip.

10:24AM N14.00011 Absence of persistent spin transport. NOAH BRAY-ALI, Physics Department, University of Southern California, ZOHAR NUSSINOV, Physics Department, Washington University, ALEXANDER BALATSKY, Los Alamos National Laboratory — A system that is in its ground state does not transport charge. Spin transport also does not occur. We extend Bohm’s argument for the absence of persistent charge transport to show the absence of persistent spin transport.

10:36AM N14.00012 Effect of Annealing on Extraordinary Hall Effects in Sputtered Granular Cu$_8$Co$_{20}$ Thin Films. NAM H. WANG, JIAN-QING WANG, SUNY-Binghamton — This work explores the microstructure dependence of extraordinary Hall effect (EHE) in Cu$_8$Co$_{20}$ granular thin films. Upon annealing, the Cu-Co films showed anomalous microstructure evolution into two-particle distribution, as evident in measured magnetic susceptibility versus temperature, showing existence of double peak structures in magnetic blocking for annealing temperature above 300 °C. Such unusual nanostructure directly affected the magneto-transport properties, most noticeable in the extraordinary Hall effect (EHE). The measured EHE was compared with Co-Ag films series, with more uniform particle distribution, which was shown to inversely scale with the scattering length and average particle sizes. Such scaling relationship was absent in Cu-Co films. It was concluded that the EHE in Cu-Co annealed films primarily depends on the population of smaller-sized particles. This was evident in independence of EHE saturation field on the annealing temperature. The gradual decrease of EHE with the annealing is a result of two combined effects. The initial linear decrease below 250 °C in EHE is a result of interface change of the Co particles in Cu matrix. As the larger particles began to emerge, further decline in EHE is due to the reducing smaller particle population, while the larger particles do not contribute significantly to the EHE.

10:48AM N14.00013 Evidence for a disorder-dependent localization correction to the anomalous Hall conductance of ultrathin Fe films. RAJIV MISRA, ARTHUR F. HEBARD, Department of Physics, University of Florida, FL 32611 — We present an experimental study of quantum corrections to the conductivity tensor of thin ferromagnetic films when the disorder is systematically varied. Using the sheet resistance as a measure of disorder, in situ magnetotransport studies were performed on a series of thin iron films deposited onto sapphire substrates having sheet resistance $R_0 \equiv R_{ee}(5K)$ varying over the range 140 $\Omega$ to 6250 $\Omega$ ($<20 \, \Omega$). For temperatures $T < 20 \, \text{K}$, a logarithmic temperature dependence of the longitudinal $R_{xx}$ and anomalous Hall resistances $R_{xy}^H$ is observed. In the low disorder limit ($R_0 < 150 \, \Omega$), we find that relative changes in the anomalous Hall conductivity $\delta \sigma_{xy}^H / \sigma_{xy}$ exhibit a temperature independent behavior implying that there are no quantum corrections to $\sigma_{xy}^H$. As disorder increases, a finite logarithmic temperature dependence to $\delta \sigma_{xy}^H / \sigma_{xy}$ appears and then evolves toward a universal weak localization correction defined by the equality $\delta \sigma_{xy}^H / \sigma_{xy} = -8R_{xy}^H / R_{xy}$ [1]. Thus with increasing disorder, we see a crossover from a region where there are no quantum corrections to $\sigma_{xy}^H$ to a region dominated by weak localization corrections. These results for iron, where spin is carried by itinerant electrons, will be compared with data on thin films of gadolinium, a localized moment system. [1] Mitra P. et al. cond-mat 0606215 (2006)

Wednesday, March 7, 2007 8:00AM - 11:00AM –
Session N16 GMAG DCOMP DMP: Focus Session: Spin and Magnetization Dynamics Colorado Convention Center Korbel 4F

8:00AM N16.00001 Ab-initio calculation of electron-phonon coupling for spin relaxation in metals. MIGUEL PRUNEDA, UC Berkeley & ICMAB, IVO SOUZA, UC Berkeley — Spin-electronic devices have motivated an important effort in understanding the mechanisms for spin-relaxation, because the operation of such devices requires long spin-diffusion lengths. Two main factors contribute to spin relaxation: (i) spin-orbit interaction, which mixes the spin-up and spin-down components of the electronic wavefunction, and (ii) electron scattering from defects or phonons. In metals, the phonon-mediated Elliot-Yafet mechanism is believed to be dominant. Realistic calculations are computationally demanding requiring an accurate description of the electronic states near the Fermi surface and their coupling to the lattice (phonons). Here we use a Density Functional Perturbation Theory implementation to calculate from first-principles the electron-phonon interaction in systems with spin-orbit coupling. Combined with recently-developed Wannier-interpolation methods for sampling efficiently the Brillouin zone, this will allow for a fully ab-initio calculation of the spin relaxation in metals.


8:12AM N16.00002 Gilbert damping and spin Coulomb drag in a magnetized electron liquid with spin-orbit interaction. EWELINA HANKIEWICZ, GIOVANNI VIGNALE, University of Missouri-Columbia, YAROSLAV TSERKOVNYAK, University of California, Los Angeles — We present a microscopic calculation of the Gilbert damping constant for the magnetization of a two-dimensional spin-polarized electron liquid in the presence of intrinsic spin-orbit interaction. First we show that the Gilbert constant can be expressed in terms of the auto-correlation function of the spin-orbit induced torque. Then we specialize to the case of the Rashba spin-orbit interaction and we show that the Gilbert constant in this model is related to the spin-channel conductivity. This allows us to study the Gilbert damping constant in different physical regimes, characterized by different orderings of the relevant energy scales – spin-orbit coupling, Zeeman coupling, disorder, $e-e$ interaction, spin precession frequency – and to discuss its behavior in various limits. Particular attention is paid to interaction effects, which enter the spin conductivity via the spin Coulomb drag coefficient.

2Project supported by NSF Grant No. DMR-0313681.
ERIC ROMAN, IVO SOUZA, University of California, Berkeley, JONATHAN YATES, Cambridge University, United Kingdom — Energy states of nonmagnetic metals may be chosen to be purely spin up and down in the absence of spin-orbit coupling. Spin-orbit coupling mixes the two states by a small amount \( b^2 \). A spin-conserving interaction (e.g. electron-phonon) causes transitions between the two states, and flips the electron’s spin. Some insight into this Elliot-Yafet spin relaxation mechanism can be obtained by averaging \( b^2 \) over the Fermi surface. In trivalent metals, such as aluminum, \( b^2 \ll 1 \) almost everywhere on the Fermi surface, except at small “hot spot” regions. Although the small regions of large \( b^2 \) dominate the spin relaxation process, they are difficult to capture numerically. We describe a Wannier interpolation strategy to compute \( \langle b^2 \rangle \). We validate it by performing \textit{ab initio} calculations on aluminum, finding good agreement with previous results.1 We also discuss interpolating \textit{ab initio} electron-phonon matrix elements to compute the spin relaxation rate.


8:36AM N16.00004 Berry phase Chern number spin Hamiltonians for nanomagnets using DFT techniques1, CARLO MARIA CANALI, Div. of Physics, Dept. of Natural Sciences, Kalmar University, Sweden. — We will present a formalism capable of describing the low-energy spin dynamics of ferromagnetic metal nanoclusters consisting of up to a few tens of atoms[1]. Our procedure is based on a quantum action with a single magnetization-orientation degree of freedom corresponding to the direction of the Kohn-Sham spin-density functional theory wave-function. Besides the magnetic anisotropy energy functional, the action contains a Berry phase term arising when the fast electronic degrees of freedom are integrated out. The associated Berry curvature has a nontrivial dependence on magnetization orientation when spin-orbit interactions are included; its average over all magnetization directions is a topological invariant known as Chern number, which can only be a multiple of half integers. From the magnetic anisotropy energy and Berry curvature functional, it is possible to construct an effective quantum Hamiltonian for the nanomagnet, in terms of a single giant-spin degree of freedom whose magnitude is equal to the Berry phase Chern number. We illustrate this procedure by computing within DFT the anisotropy energy and Berry curvature for small clusters of transition metal atoms, from which we extract the corresponding spin Hamiltonians. We show that the Berry phase term can profoundly alter the dynamics of the spin degree of freedom. Our approach can address the spin dynamics of small nanomagnets, which is now accessible experimentally in STM-engineered magnetic clusters[2].


9:12AM N16.00005 Gauge fields, the Berry phase, motive forces and the dynamics of domain walls etc., STEWART BARNES, Physics Dept., Univ. of Miami, JUN-ICHI IEDA, SADAMICHI MAEKAWA, IMR, Tohoku University — The theory of dynamics of domain walls and spin valves is described within the Stoner model. Using principally domain walls as examples, to be outlined are issues which arise beyond the traditional single electron approach to this simplest model. The (majority/minority electron) spin derived forces arise from the requirements of energy conservation and the nature of relaxation within such a simple model. While they are not currently common currency for the dynamics of domain walls and spin valves is described within the Stoner model. Using principally domain walls as examples, to be outlined are issues which arise from such dynamics are given by

\[
\vec{f}_s = \frac{\hbar}{2} \partial_{\vec{A}^+} - \nabla s \vec{r}_s^+.
\]

where the vector potential \( \vec{A}^+ \), introduced here, reflects the Berry phase and corresponds to a “no name” non-conservative spin forces. The usual “Stern-Gerlach” forces correspond to the second term. This and a second gauge field \( \vec{A} \) are required if the dynamical version of the Stoner theory is to conserve energy and angular momentum. The effects are not small and have significant experimental consequences and device applications.

9:24AM N16.00006 Topology of composite domain walls in magnetic nanostrips1, O. TCHERNYSHYOV, O. TRETIAKOV, Johns Hopkins University, YA. B. BAZALIY, Leiden University & University of South Carolina, D. CLARKE, Johns Hopkins University — We discuss the internal structure of domain walls in thin magnetic nanostrips of submicron width. The walls are composite objects made from elementary topological defects. These defects are characterized by two topological charges: the O(2) vortex winding number [1] and the O(3) skyrmion number. The defects are ordinary vortices and antivortices in the bulk and fractional vortices with half-integer winding numbers at the edge. Topology and energetics restrict the allowed compositions of a domain wall to a halfvortex and an antihalfvortex (a transverse wall) or a vortex and two antihalfvortices (a vortex wall). We present a variational model [2] that reproduces quite well the major features of a vortex wall. Despite the apparent complexity, the wall has a rigid structure. Its main degrees of freedom are the location of the vortex core and the out-of-plane magnetization of the core, which is related to the skyrmion number of the vortex. [1] O. Tchernyshyov and G.-W. Chern, Phys. Rev. Lett. 95, 197204 (2005). [2] H. Youk et al., J. Appl. Phys. 99, 08B101 (2006).

1 This work was supported in part by the NSF Grant DMR-0520491 and by the TIPAC at JHU.

9:36AM N16.00007 Dissipative dynamics of composite domain walls in magnetic nanostrips1, O. TRETIAKOV, Johns Hopkins University, YA. B. BAZALIY, Leiden University & University of South Carolina, O. TCHERNYSHYOV, Johns Hopkins University — We discuss the dynamics of domain walls in thin magnetic nanostrips of submicron width under the action of magnetic field. Once the fast precession of magnetization is averaged out, the dynamics reduces to purely dissipative motion where the system follows the direction of the local energy gradient (Glauber’s Gerlach” forces correspond to the second term. This and a second gauge field \( \vec{A}^+ \) are required if the dynamical version of the Stoner theory is to conserve energy and angular momentum. The effects are not small and have significant experimental consequences and device applications.

1 This work was supported in part by the NSF Grant DMR-0520491 and by the TIPAC at JHU.
9:48AM N16.00008 First-principles laser-driven magnetic switching scenario in NiO. GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, Kaiserslautern University of Technology — The dispersionless discrete intragap d-character levels of the (001) surface and the bulk of NiO can be selectively addressed by laser pulses and thus serve as intermediate levels for a Lambda-based all-optical magnetic switching scenario [1]. To this goal the existence of spin-mixing terms in the Hamiltonian of the system is essential, in our case it is the spin-orbit coupling term in combination with a static external magnetic field. We compute from first principles the aforementioned intragap levels with high-level correlated quantum chemistry on a doubly embedded cluster model [2] and we propagate the population in time under the influence of the laser field. The polarization, duration, shape and geometrical dependencies on the laser pulse as well as the influence of the static magnetic field are shown, and the importance of going beyond the electric dipole approximation is discussed. [1] R. Gómez-Abal, O. Ney, K. Satishkumar and W. Hübner, Phys. Rev. Lett. 92, 227402 (2004) [2] G. Lefkidis and W. Hübner, Phys. Rev. Lett. 95, 77401 (2005).

10:00AM N16.00009 Atomistic simulations of domain wall dynamics in magnetic wires1. MARIA STAMENOVA, School of Physics, Trinity College, Dublin, Ireland, TCHAVDAR TODOROV, School of Mathematics and Physics, Queen’s University of Belfast, Belfast BT7 INN, UK, STEFANO SANVITO, School of Physics, Trinity College, Dublin, Ireland — The dynamical interplay between the conduction electrons and magnetization in mesoscopic magnetic structures generates interesting new physics. For instance, there is the possibility of a domain wall (DW) motion, driven by a spin-polarized electron flux. Here we address computationally the reverse phenomenon, namely, the generation of an electromotive force (emf) by the motion of a domain wall. We describe a one-dimensional magnetic wire within the s-d model, where conduction electrons are locally exchange coupled to classical magnetizations. For this closed quantum-classical spin-polarized system we have developed an Ehrenfest Molecular Dynamics simulation, which allows us to study the spatial and temporal evolution of any observables, characterizing the system. We have studied the motion of DWs in magnetic field as function of their thicknesses (ranging from the physical limit of one atomic spacing to two orders of magnitude thicker). For all of those we have systematically found charge redistribution along the wire, governed by the DW motion, which is a signature of an emf.

1This work is supported by the Higher Education Authority, Ireland.

10:12AM N16.00010 Magnetization induced by an acoustic wave , SIMON KOS, PETER LITTLEWOOD, University of Cambridge, DARRYL SMITH, Los Alamos National Laboratory — We predict that in a semiconductor with a Rashba-type spin-orbit coupling to strain, an acoustic wave will induce a wave of magnetization. We study the effect in the ballistic and diffusive regime, and we estimate its magnitude.

10:24AM N16.00011 Effects of surface waves on crystals of molecular magnets: Semi-classical approach.1. CARLOS CALERO, EUGENE CHUDNOVSKY, Department of Physics and Astronomy of Lehman College (CUNY) — The effect of surface waves on the spin-state of a molecular magnet is theoretically investigated. As it was recently noted, the anisotropy axis of a molecular magnet is locally defined, so that its direction is modified by local distortions of the lattice. Therefore, its spin-Hamiltonian must be generally written as $\mathcal{H} = \mathcal{H}_A + \mathcal{H}_Z + \mathcal{H}_B$, where $\mathcal{H}_A = \frac{1}{2} \nabla \times u(r)$ is the angle of the local rotation induced by the displacement field $u(r)$, $\mathcal{H}_Z$ is the anisotropy Hamiltonian and $\mathcal{H}_B$ is the Zeeman term. Based on this idea we obtain the Hamiltonian describing the interaction between spin and the distortion of the lattice produced by the surface waves. We then analyze the spin-dynamics of a single nanomagnet by employing a semi-classical approach: the displacement field $u(r)$ is treated as a continuous classical field, whereas the state of the nanomagnet is described quantum-mechanically. Analytical formulas for the spin-dynamics are given for certain geometrical arrangements.

1Work supported by the NSF Grant No. EIA-0310517

10:36AM N16.00012 Ferromagnetism and current-controlled magnetization of nanomagnets with giant magnetic anisotropy , BANG-GUI LIU, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China & Beijing National Laboratory for Condensed Matter Physics, Beijing 100080, — Because the giant uniaxial magnetic anisotropy is advantageous in keeping the spins stable for practical applications in information processing and storage, we study ferromagnetism of nanomagnets with giant uniaxial magnetic anisotropy and how to control their magnetization by injecting a spin-polarized current. The giant anisotropy leads to a barrier for reversing a spin. We use kinetic Monte Carlo method to simulate the spin dynamics. We obtain the experimental ferromagnetism and its temperature dependence with experimental parameters. The ferromagnetism is formed because the nanomagnets are limited in space and the experimental duration is finite in time. Furthermore, we design a special nanomagnet and study its magnetization reversal under applied spin-polarized currents. We observe a hysteresis loop against the current. Starting from whatever value, the magnetization can be controlled by the spin-polarized current. Y Li and B-G Liu: Phys. Rev. Lett. 96, 217201 (2006); Phys. Rev. B 73, 174418 (2006).

10:48AM N16.00013 Strain and Stress in nano-structure spintronics devices due to spin transfer torque. , HAO YU, JUN-MING LIU, Nanjing National Laboratory of Microstructure, Nanjing, China — There have been many interests of the effect of magnetization reversal induced by current in spintronics, namely, spin transfer or spin torque effect, firstly predicted by Slonczewski and Berger in 1996. Because of the conservation of angular momentum in the spin transfer process, an additional lattice angular momentum has to be brought to balance the additional orbital momentum. The lattice angular momentum introduces strain and stress to the nano structure of a spintronics device. In this theoretical work, we calculate the strain and stress tensors due to spin transfer in two kinds of structure: a giant magnetoresistive (GMR) sandwich structure and a ferromagnetic nanowire. When high-density current (above some threshold value) is through them and then the named spin transfer torque effect occurs, the strain and stress in both longitudinal and transverse direction of the structure appear. We obtain the relationship between the strain tensors and magnetization in mesoscopic magnetic structures generates interesting new physics. For instance, there is the possibility of a domain wall (DW) motion, driven by spin-polarized electron flux. Here we address computationally the reverse phenomenon, namely, the generation of an electromotive force (emf) by the motion of a domain wall. We describe a one-dimensional magnetic wire within the s-d model, where conduction electrons are locally exchange coupled to classical magnetizations. For this closed quantum-classical spin-polarized system we have developed an Ehrenfest Molecular Dynamics simulation, which allows us to study the spatial and temporal evolution of any observables, characterizing the system. We have studied the motion of DWs in magnetic field as function of their thicknesses (ranging from the physical limit of one atomic spacing to two orders of magnitude thicker). For all of those we have systematically found charge redistribution along the wire, governed by the DW motion, which is a signature of an emf.

1Work supported by the NSF Grant No. EIA-0310517

Wednesday, March 7, 2007 8:00AM - 11:00AM – Session N24 DPOLY DMP: Organic LEDs and Light Emission Colorado Convention Center 201

8:00AM N24.00001 Green polariton photoluminescence in organic microcavities containing the red-emitting phosphor PtOEP. STEPHANE KENA-COHEN, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, STEPHEN R. FORREST, Department of EECS and Physics, University of Michigan, Ann Arbor, MI 48109 — Green upper and lower branch polariton photoluminescence (PL) is observed in microcavities containing the red-emitting organic phosphor 2,3,7,8,12,13,17,18-octacetyl-21H, 23H-porphyrin platinum(II) (PtOEP). This PL is attributed to cavity polariton states formed by coupling to the Q(0,0) transition of PtOEP (fluorescence). The PL spectra mirror the polariton dispersion obtained from angle-resolved reflectivity measurements. The increased fluorescence intensity compared to the neat film case is due to the reduced lifetime of the polariton states. This PL is also accompanied by strong red emission (phosphorescence) due to intersystem crossing (ISC) to the triplet state of PtOEP.
8:12AM N24.00002 Morphology, structure and photoluminescence properties of thin films of a conjugated polymer poly(2,5-dinonyl para phenyleneethynylene) . CRAIG SZYMANSKI, YUNFEI JIANG, JASSON MCNILLE, DVORA PERAHIA, Department of Chemistry, Clemson University, Clemson, South Carolina, 29634-0973, UWE H. F. BUNZ, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta GA — Poly(para phenyleneethynlenes) (PPE), are inherently semiconductor and their electro-optical characteristics depends among other factors on their association mode. PPE molecules were trapped on the surface from molecular solutions, aggregates and gels. When cast from toluene solutions bellow the critical micellar concentration (CMC) of the polymers, small clusters with an average diameter of the molecular length were observed. When cast from gel phases, a supra molecular structure that consists of well defined associating rods were detected. All of these association modes emit at 460nm. Further emissions are detected as the structure evolves from collapsed single molecules to supramolecular structure where for small non interacting rods, feature at 511 in observed and for associating rods it shifts to 550nm. Further studies are currently underway to correlate the fluorescence patterns with the structural features.

8:24AM N24.00003 Photoemission study of tris(8-hydroxyquinoline) aluminum/aluminum oxide/tris(8-hydroxyquinoline) aluminum interface . HUANJUN DING, SERKAN ZORBA, YONGLI GAO, Department of Physics and Astronomy, University of Rochester, LIPTING MA, YANG YANG, Department of Materials Science and Engineering, University of California — The evolution of the interface electronic structure of a sandwich structure involving aluminum oxide and tris(8-hydroxyquinoline) aluminum (Alq), i.e. (Alq/AlOₓ/Alq), has been investigated with photoemission spectroscopy. Strong chemical reactions have been observed due to aluminum deposition onto the Alq substrate. The subsequent oxygen exposure releases some of the Alq molecules from the interaction with aluminum. Finally, the deposition of the top Alq layer leads to an asymmetry in the electronic energy level alignment with respect to the AlOₓ interlayer.

8:36AM N24.00004 Hybrid Organic/Inorganic Semiconductor Structures: Efficient Förster Energy Coupling and Prospective Optical Devices1 . DONAL BRADLEY, Blackett Laboratory, Imperial College London, London SW7 2AZ, UK — Hybrid organic/inorganic semiconductor structures offer the prospect of combining the favourable electrical and optical characteristics of each to achieve desirable new device functions. They also provide a test bed to study the exciton state interactions between these distinct semiconductor varieties and the resultant energy transfer processes that occur between them. In this talk I will describe work on conjugated polymer/GaN structures for which efficient non-radiative Förster transfer can be achieved from the inorganic quantum well excitons to the organic (polymer) excitons. I will also discuss the prospects for optical devices based on this and related hybrid systems.

1Supported by the Research Councils UK Basic Technology Programme, the UK Engineering and Physical Sciences Research Council Ultrafast Photonics Collaboration and the Commission of the European Community IHP Network HYTEC.

9:12AM N24.00005 Study of thermal degradation of organic light emitting device structures by X-ray scattering1 , YOUNG JOO LEE, HEEJU LEE, YOUNGSUK BYUN, SANGHOON SONG, JE-EUN KIM, DAEYONG EOM, WONSUK CHA, HYUNJUNG KIM, Dept. of Physics & Interdisciplinary Program of Integrated Biotechnology, Sogang University, Korea, SEONG-SIK PARK, Orion OLED, Korea, JINWOO KIM, Department of Materials Science and Engineering, GIST, Korea — We report the process of thermal degradation of organic light emitting devices (OLEDs) having multilayered structure of [LiF/tris-(8-hydroxyquinoline) aluminum (Alq3)/N,N’-Bis(naphthalen-1-yl)-N,N’-bis(phenyl)benzidine (NPB)/copper phthalocyanine (CuPc)/indium tin oxide (ITO) /SiO₂ on a glass] by synchrotron X-ray scattering. The results show that the thermally induced degradation process of OLED multilayers is undergone several evolutions due to thermal expansion of NPB, intermixing between NPB, Alq3, and ITO layers, dewetting of NPB on CuPc, and crystallization of NPB and Alq3 depending on the annealing temperature. The crystallization of NPB appears at 1800C, much higher temperature than the glass transition temperature (Tg = 960C) of NPB. The results are also compared with findings from the atomic force microscope (AFM) images.

1Supported by Korea Science & Engineering Foundation and Seoul Research and Business Development Program (10816)

9:24AM N24.00006 Luminescence from single colloidal nanocrystals embedded in organic light emitting devices . AUGUST DORN, HAO HUANG, Department of Chemistry, Massachusetts Institute of Technology, VLADIMIR BULOVIC, Laboratory of Organic Optics and Electronics, Massachusetts Institute of Technology, MOUNGI BAWENDI, Department of Chemistry, Massachusetts Institute of Technology — The photophysical properties of individual CdSe/ZnS (core/shell) nanocrystals embedded in the active layers of electrically driven organic light emitting devices (OLEDs) were investigated at room temperature. Emission from the same nanocrystals was recorded under laser illumination and when the OLED was driven electrically. For both types of excitation we observed blinking and spectral diffusion, key signatures of single quantum dot fluorescence. Enhanced electroluminescence from the organic at the sites of nanocrystals suggests the formation of current channels through the quantum dots. This hypothesis is supported by atomic force microscopy studies of the organic layers.

9:36AM N24.00007 Charge injection and Raman scattering studies from polyfluorene-based light-emitting diodes1 , M. ARIF, S. GUHA, Dept. of Physics, University of Missouri-Columbia — Efficient and well balanced injection of charge carriers and transport capabilities are of particular importance for high luminescence efficiency in organic light-emitting diodes. Polyfluorene (PF) conjugated polymers have received widespread attention due to their strong blue emission, high charge mobility and excellent chemical and thermal stability which creates great prospect for optoelectronic device applications. Although ethyl-hexyl substituted PF (PF2/6) has a high level of molecular disorder, charge injection in single layer polymer devices can be described very well by space-charge-limited conduction for a discrete set of trap levels. This is attributed to the nature of ordering in the polymer. PFs are characterized by a number of Raman-active peaks originating from C-H bending and C-C stretching type motion. We further analyze our working devices using Raman scattering in the presence of photogenerated carriers. The Raman intensities in the 1000-1250 cm⁻¹ corresponding to a C-H bend-type motion quench in the presence of carriers with increasing fields. This effect most probably arises due to the interaction of phonons and free carriers.

1This work was supported by NSF-ECS # 0523656
9:48AM N24.00008 Multi-walled carbon nanotube sheets as transparent anodes in organic light-emitting diodes. CHRISTOPHER WILLIAMS, RAQUEL OVALLE ROBLES, MEI ZHANG, The University of Texas at Dallas, SERGEY LI, Plettronics, Inc., RAY BAUGHMAN, ANVAR ZAKHIDOV, The University of Texas at Dallas — Carbon nanotubes have emerged as useful components for next-generation electronic devices. We have investigated one such area by producing organic light-emitting which transparent multi-walled carbon nanotube sheets as a replacement for indium tin oxide (ITO). These sheets offer high optical transparency with the additional advantage of being very flexible with no loss in conductivity, making them ideal candidates for devices built on plastic substrates. We have produced devices on both high quality display glass and plastic substrates and have observed bright emission with efficiencies which are comparable to those obtained from ITO-based devices. We also present results for devices which combine ITO and nanotube sheets. Such devices take advantage of the planar conductivity of the ITO and improved injection from the nanotube sheets. We show improved efficiency in plastic devices which use this bilayer anode structure. Our results also demonstrate the importance of using a planarization layer on top of the carbon nanotube sheet to eliminate sources of leakage current. Lastly, we propose alternative device architectures such as transparent and inverted structures.

10:00AM N24.00009 Conformations in di-octyl substituted polyfluorene: a combined theoretical and experimental Raman scattering study1, 2. C. VOLZ, M. ARIF, S. GUHA, Dept. of Physics, University of Missouri-Columbia — The structural properties of polyfluorenes (PF) are extremely sensitive to the choice of functionalizing side chains. Di-octyl substituted PF (P8O2) adopts metastable structures that depend upon the thermal history and choice of solvents used in film forming conditions. We present a detailed study of the changes in the backbone and side chain morphology in P8O2, induced by the various crystallographic phases, using Raman scattering techniques. The vibrational frequencies and intensities of fluorene oligomers are calculated using hybrid density-functional theory with a 3-21G* basis set. The alkyl side chains are modeled as limiting conformations: all anti, anti-gauche-gauche, and end gauche representations. The calculated vibrational spectra of single chain oligomers in conjunction with our experimental results demonstrate the β phase, which is known to originate in regions of enhanced chain planarity, as a direct consequence of the alkyl side chain conformation.

1This work was supported by NSF-ECS # 0523656

10:12AM N24.00010 Influence of Environment on the Electronic Structure of Polyfluorenes1. ELIZABETH M. LUPTON, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112 USA — The influence of the structure of polyfluorene molecules on their emissive characteristics, as utilized in polymer LEDs, can be characterized using first principles methods. Here we concentrate on how factors such as external restrictions, structural and chemical defects, and constraints caused by side groups can affect the electronic structure of polyfluorenes, in particular the extent of conjugation along the backbone. Using Car — Parrinello Molecular Dynamics simulations, where the electronic structure is calculated according to Density Functional Theory 'on the fly' for a molecular dynamics trajectory, we systematically investigate how curving the backbone combined with torsional rotation between repeat units, as well as ketone defects, can affect the electronic structure. This demonstrates the way in which restrictions imposed by the environment could ultimately affect the light emitting properties of the polymer.

1Acknowledgement: University of Utah, DOE

10:24AM N24.00011 NEXAFS measurements of chain alignment in order polyfluorene thin films1, 2. XIAOSONG LIU, HYEUNSEOK CHEUN, University of Wisconsin, FRANK GALBRECHT, University of Wuppertal, F. J. HIMPEL, University of Wisconsin, ULLRICH SCHERF, University of Wuppertal, MICHAEL WINOKUR, University of Wisconsin — Carbon K-edge near edge X-ray absorption fine structure (NEXAFS) has been used to characterize the uniaxial surface chain alignment within the top surface (2-3 nm) of poly[bis(2-ethyl)hexyl]fluorene] thin films spin-cast atop rubbed polyimide templating substrates before and after thermal annealing. The film thicknesses range from approximately 25 to 130 nm. In the thinnest films appreciable chain alignment extends through to the top surface prior to annealing. Thermal annealing produces comparatively high levels of surface chain alignment in all film thicknesses despite a drop in the dichroic ratios, as measured by polarized optical absorption spectroscopy, in the thickest films. These data support a model that exhibits a graded morphology in which the top and bottom surfaces exhibit planar, uniaxial alignment while the film interior is less well aligned and includes a proportion of homeotropic alignment.

1Support of this work by the NSF, DOE, SRC (DMR-0537588) and Research Corporation is gratefully acknowledged.

10:36AM N24.00012 Optical studies of platinum-containing conjugated polymers. MINGHONG TONG, Physics Department, University of Utah, ALESSIO GAMBETTI, TOMER DRORI, ZEEV VARDENY, Physics Department, University of Utah — We have used a variety of steady state and ultrafast spectroscopies for studying the photophysics of platinum-containing conjugated polymers, which have potential applications as the active layer of light-emitting diodes. The intrachain heavy metal Pt atom increases the spin-orbit coupling, and this influences both the intersystem crossing time, TC, and the phosphorescence emission strength. From the ps transient pump-probe photomodulation spectroscopy and emission dynamic measurements using the up-conversion technique, we find that TC for these polymers is of order of few ps; whereas the phosphorescence lifetime is of order of few microseconds.

10:48AM N24.00013 Crystalline PTCDA waveguides grown by organic molecular beam deposition. V.R. GANGLIENKA, J. MARKUS, Department of Physics, University of Cincinnati, Cincinnati, OH 45221-0011 U.S.A., H. SCHMITZER, Department of Physics, Xavier University, Cincinnati, Ohio 45207, U.S.A., H.P. WAGNER, Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221-0011 U.S.A. — During the past few decades molecular organic semiconductors have become interesting candidates for optical and opto-electronic device applications such as organic light emitting diodes (OLEDs). Of many organic materials 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) is one of the most intensively investigated organic molecule in literature. However, so far studies on PTCDA optical waveguides are very limited. We investigate various PTCDA waveguide structures by m-line spectroscopy. The waveguides are fabricated by organic molecular beam deposition (OMBD) under high vacuum. The waveguides are deposited on a pyrex substrate or on a rutile prism with an index matching film of aluminum-quinoline (Alq3). The effective indices of refraction of observed TE and TM modes are consistent with classical electromagnetic theory. The calculated thicknesses of the waveguides under investigation are compared with reflection measurements on the same samples.

Wednesday, March 7, 2007 8:00AM - 10:48AM –
Session N27 DMP DCOMP: Focus Session: Computational Nanoscience IV - Nanoparticles
Colorado Convention Center 301
8:00AM N27.00001 Evolution of Magnetism from Atoms to Crystals1. MURILO TIAGO, University of Texas at Austin — The existence of spontaneous magnetization in metallic systems is an intriguing problem because of the extensive technological applications of magnetic phenomena and an incomplete theory of its fundamental mechanisms. Clusters of metallic atoms are important in this respect as they serve as a bridge between the atomic limit and the bulk, and they can form a basis for understanding the emergence of magnetization as a function of size. In solids, ferromagnetism is understood in terms of the exchange interaction and the formation of distinct energy bands for the majority spin and minority spin channels. In clusters, energy bands are replaced with delocalized electronic orbitals, whose properties are affected by the finite size and the presence of a surface. Therefore, the size and shape of a cluster play important role in its magnetic properties. Indeed, direct measurements have indicated a strong dependence of magnetic moment with the size of the cluster, especially in iron clusters but also nickel and cobalt. Taking advantage of recent developments in computational methods for the electronic structure of nanosystems, we can now investigate in greater detail the magnetic properties of metallic clusters containing several hundreds of atoms and understand the role of size and shape. This analysis is based on first-principles density-functional theory, within the generalized gradient approximation. Numerical calculations were done in clusters containing up to 400 atoms (iron, nickel, and cobalt). Calculations are done using the PARSEC code ( www.ices.utexas.edu/parsec ). We also discuss some of the recently developed capabilities of PARSEC.

1Supported by the National Science Foundation under DMR-0551195 and by the U.S. Department of Energy under DE-FG02-89ER45391 and DE-FG02-03ER15491.

8:36AM N27.00002 Electronic and structural properties of binary Pt-Ni nanoclusters, LUIS A. PÉREZ, IGNACIO L. GARZÓN, Instituto de Física, Universidad Nacional Autónoma de México — The lowest energy structures of binary (PtNi)ₙ, (Pt₃Ni)ₙ, and (PtNi)ₙ, nanoclusters, with n=3-10 and m=3-20, modeled by the many-body Gupta potential, were obtained by using a genetic-symbiotic algorithm. These structures were further relaxed with DFT-GGA. In agreement with the experimental evidence, segregation is observed in these clusters, where the Ni atoms are mainly found in the cluster core and the Pt atoms on the cluster surface. Furthermore, it has been experimentally found that the (Pt₃Ni)ₙ, nanoalloys present a higher catalytic activity for the N₂O + H₂ reaction at low temperatures than the other compositions [1], while the contrary trend is observed in the case of the oxidation of carbon monoxide in the presence of hydrogen, where the (PtNi)ₙ, nanoparticles present a higher catalytic activity than the other ones. In order to understand these tendencies in the catalytic performance, we performed an analysis of the surface electronic structure of the bimetallic Pt-Ni nanoclusters with the mentioned compositions, by means of first-principles density functional calculations. Acknowledgments: This work was supported by CONACyT No. 43414-F. [1] Arenas-Alatorre J., Avalos-Borja M, Diaz G J. Phys. Chem. B 109, 2371 (2005).

8:48AM N27.00003 First principles studies of the geometric and electronic structure of nanoalloy Ag₃₋₄Cu₄₋₃, M. ALCANTARA ORTIGOZA, Kansas State University, T.S. RAHMAN, University of Central Florida — We present first-principles calculations of the structure and electronic density of states (DOS) for the perfect core-shell Ag₃₋₄Cu₄₋₃ nanocluster. Our results show an expansion of 0.4 A in the diameter of the cluster compared with previous results*. From the projected DOS we conclude that the 34-atom cluster has only 2 non-equivalent Cu atoms (core) and 4 non-equivalent Ag atoms (shell), confirming that this finite-size structure has D₃ᵥ symmetry. The HOMO-LUMO gap is found to be 0.77 eV, in agreement with previous results*. Comparing with Ag bulk, the valence band centroid of Ag₂₃Cu₄ presents shift of ~1.0 eV towards the Fermi energy, but a 0.5 eV shift away from it, compared with Cu bulk. The total DOS of the structure as a whole does not present valence band narrowing when compared to the bulk of either species. Individual Ag atoms show band narrowing, a positive centroid shift to lower binding energies, and a very small enhancement of the DOS at the top of the band. Electronic states of Cu atoms are greatly concentrated in two sharp peaks in the top region of their valence band. In the bottom of the band, however, copper and silver atoms hybridize in spite of their short d-wavefunctions. Charge density plots give some insight about the hybridization of electronic states between atoms. *G. Rossi et al. Phys. Rev. Lett. 93, 105503 (2004).

1Work supported in part by DOE under grant DE-FG02-03ER46058.

9:00AM N27.00004 Bond Stiffening in Small Clusters, and its Consequences, SHOBHANA NARASIMHAN, RAGHANI PUSHPA1, UMESH WAGHMARE, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — We have used density functional theory and density functional perturbation theory to compute the interatomic force constant tensors for small clusters of Si, Sn and Pb; these results have important implications for the size dependence of the elastic and thermal properties of nanosized objects. We find a clear sequence of relationships: as the size of the cluster is decreased, bonds get shorter and stiffer and vibrational frequencies higher; however the behaviour relative to the bulk depends on the coordination number of the latter. Though all the clusters we have studied are softer than the corresponding bulk, vibrational amplitudes may be enhanced or damped relative to the bulk values, and vary non-monotonically with size. Scaling relations connect results for varying sizes and different elements. These results also provide a framework for understanding recent results showing that, surprisingly, some clusters have melting temperatures that are much higher than that of the corresponding bulk material.

1Present address: SISSA, Trieste, Italy

9:12AM N27.00005 Structural Properties of Small Pd Clusters1, JOSÉ ROGAN, Universidad de Chile, GRISELDA GARCÍA, P. Universidad Católica de Chile, JUAN ALEJANDRO VALDIVIA, Universidad de Chile, RICARDO RAMÍREZ, MIGUEL KIWI, P. Universidad Católica de Chile — The properties of small Pd clusters (2 ≤ n ≤ 21) are computed by means of an unbiased search using computational space annealing (CSA). Satisfactory agreement between the results of the several methods implemented is achieved. Of special interest is the fact that different phenomenological potentials yield the same symmetry group for the lowest energy cluster geometries. Moreover, they are in general compatible with ab initio results both of our own and other already published data.

1Supported by FONDECYT, Chile under grants 1030957 (MK and JR) and 1040356 (RR).

9:24AM N27.00006 Efficient method to calculate total energies of large nanoclusters, MIN YU, University of Illinois at Urbana-Champaign, RAMPI RAMPRASSAD, GAYANATH W. FERNANDO, University of Connecticut, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — We present a computationally efficient method to calculate total energies of very large nanoclusters based on first principles electronic structure techniques. The total energy of a cluster with well-defined facets can be separated into surface, edge, and corner energies, each a function of the chemical potentials, in addition to bulk contributions. Using density functional calculations we have verified that this separation describes the total energies of fcc Cu and zincblende CdSe, polyhedral clusters with up to 256 atoms. The calculated energies are then used to estimate the shapes of stable structures for large polyhedral nanoclusters. For sufficiently large clusters, only the surface and bulk terms survive. This method has been shown to be applicable to stoichiometric as well as non-stoichiometric clusters, containing polar or non-polar surfaces, and we are in the process of calculating the energies of various surfaces using total energy and energy density methods in order to predict equilibrium shapes of clusters as a function of size and chemical potentials.
9:36AM N27.00007 First principles study of coulombic correlation effect on lithium doped zinc oxide nanocrystals1, HYUNWOOK KWAK, MURILO L. TIAGO, University of Minnesota, JAMES R. CHELIKOWSKY, University of Texas — We examine the role of quantum confinement for impurities in zinc oxide nanocrystals. The electronic gap between the highest occupied level and the lowest unoccupied level for these systems will be larger than the band gap of bulk ZnO crystal owing to quantum confinement. We also expect quantum confinement to enhance correlation effects from on-site coulombic interactions, which will occur for lithium doped zinc oxide nanocrystals. We investigate the ionization energy for lithium impurities in ZnO nanocrystals and characterize the properties of the impurity levels. We assess the validity of arguments from recent experimental studies in which lithium impurities are expected to form shallow donor and acceptor, in ZnO. We use a real-space ab initio pseudopotential method to obtain — the ground state properties of an isolated nanocrystal. We use a rotationally invariant “LDA+U” scheme to model the on-site coulombic interaction of the zinc d-levels. The Hubbard U potential is rescaled for each nanocrystal using the static dielectric constant to reflect the reduced screening in a nanocrystal.

1Supported by the National Science Foundation under DMR-0551195 and by the U.S. Department of Energy under DE-FG02-06ER46286.

9:48AM N27.00008 Excitonic effects and optical properties of passivated CdSe clusters1, MARIE LOPEZ DEL PUERTO, University of Minnesota, MURILO TIAGO, JAMES CHELIKOWSKY, University of Texas at Austin — We calculate the optical properties of a series of passivated non-stoichiometric CdSe clusters using two first-principles approaches: time-dependent density functional theory within the local density approximation, and many-body methods, based on computing the self-energy in the GW approximation and solving the Bethe-Salpeter equation for optical excitations. We analyze the character of optical excitations leading to the first low-energy peak in the absorption cross-section of these clusters. Within time-dependent density functional theory, we find that the lowest-energy excitation is mostly a single-level to single-level transition. In contrast, many-body methods predict a strong mixture of several different transitions, which is a signature of excitonic effects. We also find that the majority of the clusters have a series of dark transitions before the first bright transition. This may explain the long radiative lifetimes observed experimentally for these clusters. Reference: PRL 97, 096401 (2006).

1Supported by the National Science Foundation under DMR-0551195 and by the U.S. Department of Energy under DE-FG02-06ER15760 and DE-FG02-06ER46286.

10:00AM N27.00009 Structure and Dynamics of Silicon Carbide Clusters: A Tight-Binding Adaptive Monte Carlo Application , ANTHONY PATRICK, XIAO DONG, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA 22030, THOMAS ALLISON, ANWAR HASMY, National Institute of Standards and Technology — A tight-binding parametrization for silicon carbide nanoclusters was developed based on the electronic energy surface of small clusters calculated within the generalized gradient approximation of density functional theory. This parametrization includes s and p angular momentum symmetries and parameters for the on-site, hopping and overlap matrix elements. With the aid of these new parameters, the global minima of silicon carbide clusters in the range of 10-30 atoms were discovered with the adaptive Monte Carlo Method [1]. The ATMC optimization process is fast and drives the system across configuration space very effectively reaching the global minimum in a small number of tempering events. Growth sequence, stability patterns, and temperature behavior were also obtained. [1] X. Dong and E. Blaisten-Barajas, J. of Comp. & Theor. Nanoscience, 3, 118-127 (2006).

10:12AM N27.00010 First-principles studies of isomerization processes of silicon clusters , LEONIDAS TSETSERIS, GEORGE HADJISAVVAS, SOKRATES PANTELIDES, Vanderbilt University — Nanoclusters typically exhibit a large number of isomers, often with strikingly different structural and electronic properties. Controlled growth and use of these ultrasmall particles depends, therefore, on an understanding of the atomic-scale details of inter-isomer conversions. Here we use first-principles calculations to study the isomerization kinetics of silicon clusters. Based on the results on activation energies, we infer a classification scheme for the complex phase of isomers in domains which are delineated by bond-breaking events at the outer cluster shells. Our findings are consistent with experimental measurements and they have implications for theoretical searches of low-energy cluster structures. We also present results on hydrogenation and oxidation kinetics and we discuss their relevance for pristine and functionalized silicon clusters. This work was supported in part by DOE Grant DEFG0203ER46096.

10:24AM N27.00011 Investigation of the structure and properties of vacancies in Si and Ge nano-crystals by ab initio methods1, SCOTT BECKMAN, JAMES CHELIKOWSKY, University of Texas — The production of nano-scale devices requires the ability to selectively dope nano-structures either n-type or p-type. The functionality of such devices demands that the dopant species remains in the nano-structure, and not diffuse into neighboring regions or to surfaces. The diffusivity of impurities in a crystal depends explicitly upon the self-diffusion of the host species. Understanding this requires understanding the modes of self-diffusion, and the mobility of intrinsic defects in the host crystal. Here we investigate the structure and properties of vacancies in Si and Ge nano-crystals. Using a real space pseudopotential method we study the energy of vacancies within 2 nm diameter crystals. It is observed that vacancies are naturally pulled toward the surfaces; however, in highly symmetric crystals, it is possible to trap vacancies in the center of the crystal. Once a vacancy is within 0.4 nm of the surface a bucking effect occurs, which indicates that a surface reaction will probably act to pull the vacancy to the surface.

1Supported by the National Science Foundation under DMR-0551195 and by the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760.

10:36AM N27.00012 Self-purification in semiconductor nanostructures2, GUSTAVO DALPIAN, Universidade Federal do ABC, JAMES R. CHELIKOWSKY, University of Texas — Doping semiconductors is an important process in order to develop functional devices with them. This suggests that, when dealing with semiconductor nanostructures, they should also be doped in order to broaden their possible applications. Experimentally this shows to be a very difficult task. “Self-purification” mechanisms are often claimed to make this task even more difficult, as the distance a defect or impurity must move to reach the surface of a nanocrystal is very small. Kinetic effects like this are usually invoked in order to explain this difficulty. Here we show that self-purification can be explained through energetic arguments and is an intrinsic property of defects in semiconductor nanocrystals. We find the formation energies of defects increases as the size of the nanocrystal decreases. This is due to the pinning of the impurity levels as the size of the nanocrystal decreases and experimental evidences support our argumentation. We analyze the case of Mn-doped CdSe nanocrystals and compare our results to experimental findings, proposing ways to improve their dopability.

2Supported by the National Science Foundation under DMR-0551195 and by the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760. GMD also thanks brazilian agencies FAPESP and CNPq.

Wednesday, March 7, 2007 8:00AM - 11:00AM – Session N28 DMP: Focus Session: Graphene II Colorado Convention Center 302
8:00AM N28.00001 Superconducting junctions in graphene1, PABLO JARILLO-HERERO, Columbia University — Graphene, a single sheet of graphite, is a two-dimensional material which has been long-studied theoretically, but only recently become available to experimentalists. Recent experiments have shown that the electronic properties of graphene are even more remarkable than previously thought. In my talk I will describe the fabrication and characterization of graphene devices, and introduce their basic electronic properties. I will then focus on our recent experiments where we study induced superconductivity in graphene, an observation which elucidates on the quantum coherent properties of electrons in this novel two-dimensional electron gas.


8:36AM N28.00002 Mesoscopic Electron Transport in Nanostructured Graphene, BARBAROS OEZ-YILMAZ, D. EFETOV, K. BOLOTIN, M. Y. HAN, P. JARILLO-HERERO, P. KIM, Physics Department, Columbia University — We present experimental results on low energy electric transport studies in mesoscopic graphene quantum devices. Graphene sheets have been fabricated by means of micromechanical exfoliation. Subsequently we define mesoscopic Aharonov-Bohm (AB) rings. The electron interference in such ring shaped graphene ribbons is controlled using a perpendicular magnetic field. We will discuss magneto-resistance oscillations obtained on AB rings with ring width of ~ 50 nm and ring diameters ranging from 300 nm to 3000 nm as a function of both temperature and carrier density. In addition, we present our efforts on locally controlling the carrier density in graphene sheets. The latter are patterned into ribbons of ~ 100nm width and contacted in a first step with source and drain electrodes. In a second step multiple lithographically patterned electrostatic local top gates are attached to each device. We will discuss transport measurements as a function of local gate voltages.

8:48AM N28.00003 Observation of Proximity Effect and Multiple Andreev Reflections in Graphene/Superconductor Junctions1, XU DU, IVAN SKACHKO, EVA Y. ANDREI, Dept. of Physics, Rutgers University — Graphene, a single atomic layer of graphite, has attracted much interest recently both for its unique physical properties and for its potential in electronics applications. Due to the combined effects of a linear energy-momentum dispersion and internal degrees of freedom (pseudo-spin) associated with the honeycomb lattice, the low energy excitations in graphene are expected to behave like massless relativistic fermions. This leads to many novel and unusual physical properties. We will present experimental studies on a gate controlled superconductor/graphene hybrid device. Electric field dependent superconducting proximity effect and multiple Andreev reflections will be discussed. Results obtained for junctions fabricated on graphene and on multi-layer graphite films will be compared.

1Work supported by NSF-DMR-0456473 and by DOE DE-FG02-99ER45742

9:00AM N28.00004 Quantum Transport in Single and Bi-Layer Graphene Coupled to Superconducting Electrodes, F. MIAO, S. WIJERATNE, U. COSKUN, Y. ZHANG, C. N. LAU, Department of Physics and Astronomy, University of California, Riverside, CA 92521 — Graphene, the two dimensional honeycomb lattice of carbon atoms, has attracted significant attention in recent years, due to its unique electrical properties. Here we present experimental studies of single and bi-layer graphenes coupled to superconducting electrodes. At low temperatures the devices display signatures of ballistic electrical transport, and the minimum conductivity varies between 6.5 and 20kΩ. When the electrodes become superconducting, we observe gate-tunable low-bias conductance peaks, which are attributed to multiple Andreev reflections. Latest experimental results will be discussed in terms of various theoretical models.

9:12AM N28.00005 Low Field Electronic Transport Properties and Scattering Mechanisms of Graphene, Y.-W. TAN, Columbia Univ., Y. ZHANG, UC Berkeley, M. HAN, Columbia Univ., J. A. JASZCZAK, Michigan Technological Univ., P. KIM, Columbia Univ., H. L. STORMER, Columbia Univ. and Bell Labs, Lucent Technology — We report low magnetic field transport properties of fourteen graphene devices with a wide spread of mobilities. The minimum conductivity at the Dirac point lies in the range 2 – 12e²/h with an average of ~ 8e²/h. When compared to the low mobility samples, the high mobility samples show the features characteristic of short range scattering and low mobility samples show the features characteristic of long range scattering. Samples exhibiting different scattering mechanisms also show different weak localization behaviors. Samples having short range disorder show total suppression of weak localization (WL), whereas samples with long range scattering show the conventional WL peak with a reduction in amplitude. Devices in between these two limits have a sharp, narrow WL peak. Under moderate disorder scattering, we find inelastic electron-electron scattering to be the major cause of phase decoherence, and the phase coherence length has a n²/4 dependence.

9:24AM N28.00006 Controlling the Electronic Structure of Bilayer Graphene, TAISUKE OHTA, AARON BOSTWICK, JESSICA MCCHESNEY, Lawrence Berkeley National Laboratory, THOMAS SEYLLER, Universitat Erlangen-Nurnberg, KARSTEN HORN, Fritz-Haber-Institut, ELI ROTENBERG, Lawrence Berkeley National Laboratory — Carbon-based materials such as carbon nanotubes, graphite intercalation compounds, fullerences, and ultrathin graphite films exhibit many exotic phenomena such as superconductivity and an anomalous quantum Hall effect. These findings have caused renewed interest in the electronic structure of ultrathin layers of graphene: a single honeycomb carbon layer that is the building block for these materials. There is a strong motivation to incorporate graphene multilayers into atomic-scale devices, spurred on by rapid progress in their fabrication and manipulation. We have synthesized bilayer graphene thin films deposited on insulating silicon carbide and characterized their electronic band structure using angle-resolved photoemission. By selectively adjusting the carrier concentration in each layer, changes in the Coulomb potential led to control of the gap between the two Dirac points. As the tunnel barrier and Pb or Au as the counter-electrode. We observed a phenomena similar to Cooper pairing instability in graphene coated with alkane and transition metals, and similar low dimensional graphene based devices.

9:36AM N28.00007 Superconductivity in metal coated graphene, BRUNO UCHOA, ANTONIO CASTRO NETO, Physics Dept, Boston University — Graphene, a single atomic layer of graphite, is a two dimensional (2D) zero gap insulator with a high electronic mobility between nearest neighbor carbon sites. The unique electronic properties of graphene, from the semi-metallic behavior to the observation of an anomalous quantum Hall effect and a zero field quantized minimum of conductivity derive from the relativistic nature of its quasiparticles. By doping graphene, it behaves between nearest neighbor carbon sites. The unique electronic properties of graphene, from the semi-metallic behavior to the observation of an anomalous quantum Hall effect and a zero field quantized minimum of conductivity derive from the relativistic nature of its quasiparticles. By doping graphene, it behaves like a metal. In our experiments, we fabricate graphene devices using an ultrathin quartz filament as a shadow mask over mechanically exfoliated graphene, and then test their electronic properties using a wide range of methods.

9:48AM N28.00008 Tunneling and Josephson coupling studies of n-layer graphene, CONOR PULS, NEAL STALEY, HAOHUA WANG, JEREMY FORSTER, KELLY MCCARTHY, BEN CLOUSER, YING LIU, Department of Physics, The Pennsylvania State University — We investigate planar tunnel and superconductor-graphene-superconductor (SGS) junctions involving n-layer graphene. We fabricate our devices using a two-step process. In the first step, we fabricate devices using a two-step process. In the second step, we use a DC pulse to remove the graphene layer. The resulting devices show a wide range of novel phenomena, such as the observation of a zero energy gap at the Fermi level, and the observation of a range of unusual transport behaviors.

Our tunnel junctions use A12O3 as the barrier layer and Pb or Au as the counter-electrode. We observed a reduction of density of states in the n-layer graphene and the superconducting energy gap of Pb when Pb was an electrode. Results from work on SGS junctions and other atomically thin materials such as NbSe2 will also be presented.
Among various synthesis methods of carbon nanotubes (CNT), catalytic CVD method has gained its majority. There are several reasons for the popularity of CVD synthesis:

1. Scale capability: CVD method is able to synthesize CNT on a large scale in a continuous and controlled process.
2. Cost-effective: Large-scale synthesis reduces the cost per unit of CNT production.
3. High purity: CVD method allows for precise control over the synthesis process, leading to high purity nanotubes.
4. Long lifetimes: The catalytic lifetime and growth rate are critical factors in determining the length and alignment of CNTs. Differences in these parameters significantly affect the size and alignment of synthesized CNTs.

In collaboration with Hiroyuki Muramatsu, Yoong Ahm Kim, and Morinobu Endo, Shinshu University and the Endo Lab Team.

In the present talk, the process of producing high quality DWCNT and its morphological changes by various treatments will be shown. We have been working with the CCVD method for producing high quality nanotubes, and by finding the right synthesis condition, succeeded in obtaining highly homogeneous double-wall carbon nanotubes (DWCNT). In the heat-treated DWCNT sample, we were able to find various coalesced tubes with two CNT morphologies controlled by substrate-graphene interaction.

We detect the thermal motion of the resonators, and use the equipartition theorem to calibrate the amplitude of motion. For example, a 5nm graphite sheet at room temperature has thermal motion on resonance of 200 fm/Hz^{1/2}, and shows a driven linear response in displacement up to 6 nm, comparable to the thickness of the resonator. The unusually small mass, electrically active material and reasonable dynamic range indicate that graphite resonators would make excellent force and charge sensors.

Tendencies toward true spin and pseudospin polarizations in graphene will also be examined. Statistical Science, LANL, ALLAN MACDONALD, University of Texas at Austin — The properties of localized states (especially states localized at the edge of ribbons) will be presented for various graphene systems. The orientation dependence of the properties will be discussed. Methods for devising appropriate boundary conditions for Dirac ribbons will be reviewed. Localization at zero field due to finite size effects, applied magnetic fields, and spin-orbit coupling will be discussed. Tendencies toward true spin and pseudospin polarizations in graphene ribbons will also be examined.
8:48AM N29.00003 Distribution and stability of Carbon in Fe-C nanoparticles.¹. NEHA AWASTHI, Duke University, USA, AIQIN JIANG, Duke University, USA, ALEKSEY KOLMÓGOROV, WAHYU SETYAWAN, Duke University, USA, KIM BOLTON, Goeteborg University, Sweden, STEFANO CURTAROLO, Duke University, USA — Catalytic Chemical Vapor deposition (CVD) method is widely used to produce carbon nanotubes. To improve our understanding of the CVD growth mechanism, we focus on the thermodynamics and the phase stability of catalyst Fe-C nanoparticles. Using ab initio methods and classical molecular dynamics simulations, we investigate 1) the diffusion and solubility of carbon atoms in nanoparticles by calculating the distribution of carbon atoms inside the clusters, 2) the formation and stability of carbides at nanoscale, and 3) the effect of substrates on such structures. We address the implications of these results on NT growth, and give possible strategies to mitigate the problems.

¹Honda Research Institute Inc., USA

9:00AM N29.00004 Challenges for Growth of Smallest Diameter Single-Walled Carbon Nanotubes by Catalytic Method. OLEG KUZNETSOV, ELENA MORA, TOSHIO TOKUNE, Honda Research Institute USA Inc., STEFANO CURTAROLO, Duke University, KIM BOLTON, Goeteborg University, AVETIK HARUTYUNYAN, Honda Research Institute USA Inc., HONDA RESEARCH INSTITUTE USA INC. TEAM, DUKE UNIVERSITY TEAM, GOTEHBORG UNIVERSITY TEAM — We investigate the viability of formation of very small diameter (< 0.5nm) freestanding SWNTs by CVD based on concept of carbon diffusion through the catalyst particle, originated from the vapor-liquid-solid growth mechanism. We found that the decrease of particle size required for nucleation of small diameter tubes results in a significant increase of catalytic decomposition temperature of hydrocarbon and, accordingly, the temperature required for nucleation and growth of nanotubes. However, high temperature increases the mobility of particles and endorses their agglomeration with formation of bigger particles, as well as leads to deactivation of catalyst by formation of intermetallic compounds with support material. The results of Raman spectroscopy, (n,m) assignments of the grown tubes and TEM studies for the smallest diameter tubes are presented. Performed ab-inito and molecular dynamics simulations qualitatively explain the experimental finding based on size dependent carbon solubility of catalyst, by analyzing supported nanocatalyst-carbon binary phase diagram.

9:12AM N29.00005 Growth of carbon nanotubes by the pyrolysis of thiophene.¹, GAOHUI DU, WENZHI LI, Department of Physics, Florida International University, Miami, FL 33199 — Branched carbon nanotubes have been reported and produced by the pyrolysis of metalloocene-thiophene mixture. In our experiments, we prepared the carbon nanotubes (CNTs) by the pyrolysis of thiophene as the carbon source over cobalt catalyst. Of the length of carbon nanotubes the length of 0.5-1 mm are obtained. The effects of flow rate and temperature on the growth of CNTs have been investigated. The branched carbon nanotubes were also found in the experiments, showing Y-junction or T-junction, even connecting each other to form a web. The growth mechanism of the branched CNTs was studied using transmission electron microscopy. The electron transportation properties along these branched CNTs are under investigation.

¹This work is supported by the NSF Career grant DMR-0548061

9:24AM N29.00006 Initial Stage of Growth of Single-Wall Carbon Nanotubes: Modeling and Simulations.¹. J. CHAUDHURI, M. YU, C. S. JAYANTHI, S. Y. WU, University Of Louisville — Through a careful modeling of interactions, collisions, and the catalytic behavior, one can obtain important information about the initial stage of growth of single-wall carbon nanotubes (SWCNTs), where a state-of-the-art semi-empirical Hamiltonian [Phys. Rev. B, 74, 155408 (2006)] is used to model the interaction between carbon atoms. The metal catalyst forming a supersaturated metal-allyl droplet is represented by a jellium, and the effect of collisions between the carbon atoms and the catalyst is captured by charge transfers between the jellium and the carbon. Starting from carbon clusters in different initial configurations (e.g., random structures, cage structures, bulk-cut spherical clusters, etc.), we anneal them to different temperatures. These simulations are performed with clusters placed in the jellium as well as in vacuum. We find that, in the presence of jellium, and for an optimal charge transfer of ~ 0.2e, open cage structures (and some elongated cage structures) are formed, which may be viewed as precursors to the growth of SWCNTs. We will also discuss the implications of a spherical boundary on the nucleation of a SWCNT.

¹Funding Sources: Honda Research Grant and KSEF.

9:36AM N29.00007 Universal Template Technique for Patterned Growth of Carbon Nanotubes. YING CHEN, HUA CHEN, JUN YU, BILL LI, VINCE CREIG, JAMES WILLIAMS, Department of Electronic Materials Engineering, The Australian National University, Canberra, ACT 0200 — A new template technique has been developed to help patterned growth of carbon nanotubes on Si surface without preposition of metal catalysts. Focused ion beam (FIB) milling system was used to create nanosized patterns on Si wafer surface as the template. Under a controlled pyrolysis of iron phthalocyanine at 1000 °C, carbon nanotubes only nucleate and grow in the template. The selective growth is due to the special surface morphology and crystalline structure created by FIB. This template technique can be used to help patterned growth of other nanotubes and nanowires on any substrates.

9:48AM N29.00008 Synthesis of Narrow Chirality Distributions of Single-Walled Carbon Nanotubes using Catalyst Particle Templates Produced by Nanosphere Lithography. NOUreddine Tayebi, Joseph Lyding, University of Illinois at Urbana-Champaign — We report a simple and inexpensive technique based on nanosphere lithography [1], which allows for the fabrication of periodically-spaced and monodispersed metal particles from which the chemical-vapor-deposition synthesis of single-walled carbon nanotubes (SWNTs) is achieved. We have controlled the diameter of these metal particles, and thus that of the SWNTs, from 1 nm down to 0.7 nm, with an interparticle spacing varying from 50 nm down to 5 nm. Raman spectroscopy analysis reveals that a narrow chirality distribution is achieved. We are currently confirming the chirality results using fluorescence spectroscopy and scanning tunneling microscopy. Transmission electron microscopy analysis reveals that the 0.7 nm particles are crystallographically identical, which could be the origin of such a narrow distribution. Furthermore, the current technique was used to grow aligned SWNTs on single-crystal quartz substrates [2]. [1] J. C. Hulteen et al., J Vac Sci Technol A, 13, 1553 (1995) [2] C. Kocabas et al., J Am Chem Soc, 128, 4540 (2006)

10:00AM N29.00009 Synthesis and characterization of dense, vertically-aligned carbon nanotube forests from 10nm colloidal iron oxide nanoparticles. David Hutchison, Brendan Turner, Richard Vanfleet, Robert Davis, Brian Woodfield, Juliana Boerio-Goates, Brigham Young University — We report growth of vertically-aligned carbon nanotubes (VANCNTs) on alumina using 10nm iron oxide nanoparticles dried from a colloid. VANCNTs were grown by chemical vapor deposition using ethylene, hydrogen and argon, and found to be dense forests with height, number of walls, and density dependent on the catalyst concentration. Comparison between VANCNTs produced from nanoparticles and those from more traditional sputtered or evaporated iron films will be made. The forests have been characterized by Raman, TEM, and SEM, and the iron catalyst particles by AFM and TEM. Growth directly from pre-prepared nanoparticles of uniform size offers insight into how the catalyst particles seed carbon nanotube growth and is easier to prepare and faster than iron film deposition by sputtering.
10:12AM N29.00010 Synthesis and Structure of Carbon Nanotube Y-junctions, BIMAL PANDEY, WENZHI LI, Department of Physics, Florida International University, Miami, FL 33172 — The effect of catalyst and carbon source on the synthesis and structure of carbon nanotube Y-junctions (CNTYs) using chemical vapor deposition has been investigated. Three different nitrates, including cobalt nitrate, calcium nitrate, and magnesium nitrate, are used as catalyst precursors and thiophene (C4H4S) is used as carbon source to synthesize CNTYs. CNTYs with straight branches are synthesized by using mixture of cobalt/magnesium nitrates or cobalt/calcium nitrates while individual cobalt nitrate, magnesium nitrate, calcium nitrate, or mixture of magnesium/calcium nitrates doesn’t grow any CNTYs, indicating that cobalt/magnesium or cobalt/calcium facilitate the formation of CNTYs. Experimental result shows that the diameter and yield of CNTYs are affected by the ratio of cobalt/magnesium or cobalt/calcium nitrates. In addition, carbon sources such as methane (CH4) and acetylacetonel (C5H7O2) have also been used as carbon source to grow CNTYs. It is found that linear nanotubes rather than CNTYs can be formed. The result shows both the catalyst and the carbon source affect the formation of CNTYs.

10:24AM N29.00011 Melting and Premelting of Carbon Nanotubes1, KAIWANG ZHANG, Xiangtan University, G. MALCOLM STOCKS, JIANXIN ZHONG, Oak Ridge National Laboratory — We report results of molecular dynamics simulations of melting and premelting of single-walled carbon nanotubes (SWNTs). We found that the traditional critical Lindemann parameter for melting of bulk crystals is not valid for SWNTs. Using the much smaller critical Lindemann parameter developed for melting of nanoparticles as a criterion, we show that the melting temperature of perfect SWNTs is 4800K. We further show that Stone-Wales defects in a SWNT significantly reduce the melting temperature of atoms close the defects, resulting in premelting of SWNTs around the defects at 2600K.

1Supported by the Education Bureau of Hunan Province, China and by the Material Sciences and Engineering Division Program of the DOE Office of Science under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

10:36AM N29.00012 Direct growth of carbon nanotubes on BaTiO3 thin films for ferroelectric field effect devices, PATRYCJA PARUCH, LASSP, Cornell University, AGHAM-BAYAM POSADAS, CHARLES H. AHN, Yale University, PAUL L. MCEUEN, LASSP, Cornell University — Carbon nanotube field effect transistors have been extensively investigated using a variety of gate dielectrics. We propose instead to use ferroelectric (FE) field effect, replacing the dielectric by a thin FE film on a conducting substrate. The remanent FE polarization can provide reversible, locally-controlled, and non-volatile electronic doping of up to ~ 5 x 1014 charges/cm2, over 10 times greater than that available with SiO2 at breakdown fields. However, many FE materials cannot withstand the high temperatures and reducing atmosphere required for CNT growth. We subjected different perovskite FEs to CNT growth conditions, and from subsequent local and macroscopic measurements of their polarization we have identified BaTiO3 as a good device material. Single walled CNTs grown on BaTiO3 were characterized using the Nb:SrTiO3 substrate as a gate electrode. The effects of FE polarization on the CNT electronic properties are currently being studied.

10:48AM N29.00013 Replicating carbon nanotubes with molybdenum chalcogenide nanowires1, TENG YANG, DAVID TOMANEK, Michigan State University, IGOR POPOV, GOTTHARD SEIFERT, TU Dresden — In an attempt to design chemically stable and easily separable one-dimensional conductors, we performed ab initio Density Functional calculations for MoS2, MoI2 nanowires with a varying concentration of iodine. Such Chevrel like systems have been synthesized before, but had necessitated alkalil counter-ions for stabilization. The backbone of our nanowires consists of Mo6 octahedra structures, covered by I and S atoms. We find the stoichiometry with x = 2 to be preferred on energy grounds. Our results suggest these nanowires to be not only structurally rigid, but also to be rather easily separable. The electronic structure of these nanowires strongly resembles that of semi-metallic carbon nanotubes, with two crossing bands giving rise to a constant density of states, flanked by a pair of van Hove singularities near the Fermi level. Since the semi-metallic nature of these nanowires is robust, these systems may offer a viable alternative to carbon nanotubes, where conductivity strongly depends on chirality.

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

Wednesday, March 7, 2007 8:00AM - 11:00AM – Session N31 DMP: Focus Session: Carbon Nanotubes: Sensors and Adsorption Colorado Convention Center 401

8:00AM N31.00001 Raman Spectroscopy in Single-Wall and Double-Wall Carbon Nanotube Systems Doped with H2SO4, EDUARDO BARROS, Tohoku University, ANTONIO SOUZA FILHO, Universidade Federal do Ceara, YOONG-ARM KIM, HIROYUKI MURAMATSU, TAKUYA HAYASHI, Shinsyu University, RICHIRO SAITO, Tohoku University, MORIBONU ENDO, Shinsyu University, MILDRED DRESSELHAUS, Massachusetts Institute of Technology — In this work we performed Raman experiments on a mixture of single-wall and Double-wall carbon nanotubes for different relative concentrations and using different laser energies. Two sets of samples were analyzed, one which was exposed to H2SO4 for 5 s and one which is pristine. The H2SO4 is known to act as an acceptor for the electrons of graphitic materials. The effect of hole doping on the vibrational and electronic properties of the double and single-wall carbon nanotubes is probed using Resonant Raman scattering with different excitation energies probing different nanotubes. For selected excitation energies, it is possible to probe, at the same time, the inner and outer walls of double-wall nanotubes. The lineshape of the G’ band double-wall nanotubes is discussed in terms of the interlayer interaction and the effect of single-wall nanotube contaminants and the H2SO4 doping to the G’ band is studied.

8:12AM N31.00002 Evidence of a possible phase transition in ethane adsorbed on purified HiPco nanotubes1, MURAT BULUT, DINESH RAWAT, ALDO MIGONE, Southern Illinois University Carbondale — We conducted adsorption measurements for ethane on purified HiPco single-walled carbon nanotubes for coverages in the first layer. In order to obtain the binding energy of ethane, we measured three low-coverage isotherms for temperatures between 220 K and 240 K. The value that we determined, 308 meV, is 1.7 times larger than that obtained for the binding energy of ethane on planar graphite. We measured eight full isotherms between 103 K and 170 K. Evidence of a phase transition in the adsorbed film was investigated by studying temperature dependence of the height of the isotherm substep corresponding to the adsorption of ethane molecules on the external surface of the SWNTs. There is a significant difference in the size of the substeps measured below and above 110 K. This difference suggests that a possible structural phase transition is occurring in the adsorbed film.

1This work was supported by the NSF through grant DMR-0089713.
8:24AM N31.00003 First Principles Study of Metal Adatom Adsorption on Carbon Nanotubes1
, KEVIN T. CHAN, University of California, Berkeley, JEFFREY B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, MARVIN L. COHEN, University of California, Berkeley and Lawrence Berkeley National Laboratory — Recent experiments observed bias-induced mass transport between indium nanoparticles on a carbon nanotube. Ab initio studies later suggested that electromigration in this case can be explained by charge transfer from indium adatoms to the nanotube and small diffusion barriers, and that defects can serve as nucleation sites for nanoparticle formation. Here we use ab initio calculations to explore adhesion, diffusion, and the possibility of mass transport on nanotube surfaces for other metallic species. We will present calculations examining binding energy, binding site, diffusion barriers, and charge transfer for a range of metal adsorbates on surfaces, defects, and vacancies of carbon nanotubes and sheets. Adatom coverage dependence and the role of curvature effects will also be discussed.

1 This work was partially supported by NSF Grant No. DMR04-39768 and by DOE under Contract No. DE-AC02-05CH11231. Computational resources were provided by NERSC and NAPCI.

8:36AM N31.00004 Accessible surface area in filter deposited, single wall carbon nanotube films1 , RAJIB K. DAS, BO LIU, RYAN M. WALCZAK, ANDREW G. RINZLER, University of Florida — A convenient process for fabricating thin, homogeneous, transparent films of single wall carbon nanotubes (SWNTs), with potential application as electrodes in organic light emitting diodes and photovoltaic devices, was described in 2004[1]. Among the advantages claimed for such films was the high surface area contact afforded by the nanotubes. Recent measurement of the density for such films shows them to possess nearly 60% of the crystallographic hexagonal close pack density for nominally 1.36 nm diameter SWNTs. Such dense packing does not bode well for infiltration of the films with viscous electro-active polymers by e.g. spin coating. Hence, while the films in principle possess large surface areas, it is not necessarily accessible. To improve this circumstance we have developed a simple, controllable method for modifying the open porosity of the films. We will describe the method and its characterization by imaging, sheet resistance and electrochemical capacitance measurements. [1] Z. Wu et al. Science 305, 1273 (2004)

1We thank NanoHoldings LLC for support of this work

8:48AM N31.00005 Gas Adsorption on Carbon Nanohorns Aggregates, JEFF WAGNER, M. MERCEDES CALBVI, Dept. of Physics, Southern Illinois University Carbondale — We evaluate a simple model of adsorption to predict the possible adsorbed phases of gases on a triangular array of tubes as a function of the distance between the tubes and the external pressure. Specific results are presented for the cases of Ne and CF4. In addition, Grand Canonical Monte Carlo simulations are performed for particular choices of the aggregates geometry. Adsorption isotherms and isostructural heats of adsorption as a function of coverage are obtained. Comparison with experimental results allows us to obtain information on the structure of the aggregates that is then use to predict the adsorption behavior of other gases.

9:00AM N31.00006 Kinetic Selectivity and Competitive Adsorption on Carbon Nanotube Bundles1 , JARED BURDE, M. MERCEDES CALBVI, Dept. of Physics, Southern Illinois University Carbondale — We investigate the kinetics of adsorption of a binary mixture on one-dimensional chains by means of Kinetic Monte Carlo simulations. A competition based on both the binding energies and the adsorption rates is demonstrated. Since the species with smaller binding adsorb faster, it is shown that before reaching equilibrium, that species is the favored one contrary to what eventually happens in equilibrium. Therefore, the weaker binding species can initially reach coverages larger than its equilibrium value, providing evidence of a kinetic selective process that can be exploited for gas separation purposes.

1Acknowledgement is made to the Donors of the American Chemical Society Petroleum Research Fund for partial support of this research.

9:12AM N31.00007 Scaffolding Carbon Nanotubes into Single-Molecule Circuity, PHILIP COLLINS, Univ. of California, Irvine — As electronic devices shrink to the nanometer scale, the relative importance of individual chemical bonds becomes larger and larger. Single-walled carbon nanotubes (SWNTs) represent an extreme limit of this rule, as the modification of a single lattice site can dramatically change chemical activity and electronic properties. This presentation will focus on single-site experimentation in which we find, create, and alter point defects in SWNTs. Due to the correspondence between chemical and electronic properties, changes in SWNT device conductance reveal these chemical processes happening in real-time and allow the SWNT sidewall to be deterministically broken, reformed, and conjugated to target species. We routinely functionalize pristine, defect-free SWNTs at one, two, or more sites, and have demonstrated three-terminal devices in which a single-molecule attachment controls the electronic response.

9:48AM N31.00008 Supported Lipid Bilayer/Carbon Nanotube Hybrids1 , XINJIAN ZHOU, Laboratory of Atomic and Solid-State Physics, Cornell University, JOSE MORAN-MIRABAL, HAROLD CRAIGHEAD, Applied and Engineering Physics, Cornell University, PAUL MCEUEN, Laboratory of Atomic and Solid-State Physics, Cornell University — We form supported lipid bilayers on single-walled carbon nanotubes and use this hybrid structure to probe the properties of lipid membranes and their functional constituents. We first demonstrate membrane continuity and lipid diffusion over the nanotube. A membrane-bound tetanus toxin protein, on the other hand, sees the nanotube as a diffusion barrier whose strength depends on the diameter of the nanotube. Finally, we present results on the electrical detection of specific binding of streptavidin to biotinylated lipids with nanotube field effect transistors. Possible techniques to extract dynamic information about the protein binding events will also be discussed.

1This work was supported by the Nanobiotechnology Center (NBTC), an STC Program of the National Science Foundation under Agreement No. ECS-9876771. JM thanks CONACyT for support through its graduate fellowship program.

10:00AM N31.00009 Carbon nanotube biosensors strongly affected by the biosensitivity of quasi reference electrodes , ETHAN MINOT, ANNE JANSSSENS, IDDO HELLER, DIRK HEERING, CEES DEKKER, SERGE LEMAY, TU Delft — Semiconductor carbon nanotubes are extremely sensitive to their electrostatic environment. This property can be utilized to build sensors in liquid environments that detect bio-molecular adsorption in real time via changes in device conductivity. Control of the liquid potential is critical for operation of these sensors, yet nearly all carbon nanotube sensors operating in liquid have employed bare Pt wire to control the liquid potential. We show that the interface voltage between Pt and an electrolyte solution changes by tens of mV upon protein adsorption. This quasi reference electrode biosensitivity can easily mask signals associated with protein adsorption around the carbon nanotube. We demonstrate stable control of the liquid potential using a standard reference electrode, and report signals due entirely to protein adsorption around individual semiconducting NTs. These improved measurements allow us to quantify and differentiate the mechanisms of protein sensing by carbon nanotube devices.
Nanotubes glycine-coated SWNT-FET have been changed to be metallic in the presence of alcohol. Using ab initio inorganic heteroepitaxy.

...direction and their aromatic planes have a significant tilt angle to the substrate arising from the weak bond to the surface and adopting the surface corrugation.

...backdonation, but are adsorbed in opposite directions: [1-10] and [001], respectively. On the full reconstructed surface the 6P molecules are pointing in [001]... 

...sub-molecular scale by using low-temperature scanning tunneling microscopes. Combined with low energy electron diffraction and first-principles density functional theory calculations, the key parameters in modulating molecular structures on metals are analyzed. It is found that the alkyl chains of quinacridone derivatives (QA) determine the orientation of molecular overlayers on an Ag(110) substrate. The interaction of QA and the Ag substrate is primarily due to chemical bonding of oxygen to specific positions at the silver substrate, determining the molecular orientation and preferred adsorption site. However, the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g. the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g.

...the absorption of oxygen to specific positions at the silver substrate, determining the molecular orientation and preferred adsorption site. However, the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g.

...the absorption of oxygen to specific positions at the silver substrate, determining the molecular orientation and preferred adsorption site. However, the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g. the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g.

...the Ag(110) substrate. The interaction of QA and the Ag substrate is primarily due to chemical bonding of oxygen to specific positions at the silver substrate, determining the molecular orientation and preferred adsorption site. However, the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g.

...the Ag(110) substrate. The interaction of QA and the Ag substrate is primarily due to chemical bonding of oxygen to specific positions at the silver substrate, determining the molecular orientation and preferred adsorption site. However, the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g. the intermolecular arrangement can be adjusted via the length of attached alkyl chains. We are thus able to fabricate uniform QA films with very well controlled physical properties. Furthermore, by thermal and chemical control, we are able to self-assemble three dimensional molecular nanostructures, e.g.

...In collaboration with D.X. Shi, S.X. Du, W. Ji, Z.T. Deng, L. Gao, Institute of Physics, and X. Lin, Chinese Academy of Sciences, China; C. Seidel and H. Fuchs, Universität Münster, Germany; W.A. Hofer, The University of Liverpool, Britain; and S. T. Pantelides, Vanderbilt University, USA.

...sensing experiments that demonstrate that sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.

...sensing is not only localized at the contacts. Furthermore, through protein adsorption experiments we show that the effect of either bulk or contact adsorption can dominate the overall electrical signal and gate potential. Because protein adsorption at bulk and contacts can have opposite effects on device conductivity, the two mechanisms can even cancel each other out. This makes it crucial to carefully choose the operating gate potential for protein sensing experiments where the device conductivity is monitored over time.
8:48AM N42.00003 Self-assembly of methanethiol on cluster arrays of Co/Au(111)¹, GEORGI NENCHEV, BOGDAN DIACONESCU, KARSTEN POHL, University of New Hampshire — Self-assembly on strained metallic interfaces is an attractive option for growing highly ordered multi-functional nanopatterns. We present a Variable Temperature STM and Auger Electron Spectroscopy study of selective adsorption of sulfur-terminated CH₃SH molecules on the lattice of Co clusters on Au(111). We investigate the growth of a uniform network of Co on the reconstructed Au(111) surface, the temperature evolution of the island height and the termination, and the onset of surface alloying. Further we will show the evolution of morphology of the CH₃SH film on Au(111) as a function of coverage and temperature, and the importance of the herringbone reconstruction for the SAM formation and orientation. Successful combination and control of these two processes leads to the creation of an ordered, stable patterned Co/CH₃SH heterostructure with nanometer-sized unit cell.

¹This work is supported under the Nanoscale Science and Engineering Centers Program of National Science Foundation (Award # NSF-0425826)

9:00AM N42.00004 An STM Study of Nucleation and Growth of Co Nanostructures on Stepped Cu(775)¹, NADER ZAKI, DENIS POTAPENKO, RICHARD OSGOOD, JR., Columbia University, PETER JOHNSON, Brookhaven National Lab — We conduct an STM study of nucleation and growth of Co nanostructures on stepped Cu(775) surface. This surface has a relatively narrow terrace width of 1.4Å between the steps. A critical mass of Co is required before condensation of clusters into stacks occurs at room temperature, while at 200°C the Co immediately forms distinguishable stacked islands. After the completion of the first monolayer, LEEM observations of this system show the development of 3D Pb crystallites, with the island density depending strongly on temperature. For Pb deposition at a substrate temperature of 200°C, the islands grow together and form larger islands with quasi-hexagonal sides. Annealing the Pb crystallites causes them to merge and reshape while maintaining long-range order. The crystallites melt at the usual Pb melting temperature of 323°C, resulting in small, round, disordered islands. Upon recooling, the islands develop a hexagonal shape. They desorb from the surface at approximately 452°C.

¹This work is funded by DOE Grant No. DE-FG02-04ER46157 “Mapping the electron response of nanomaterials”.

9:12AM N42.00005 Size dependent superconductivity of nano-sized Pb islands studied by low temperature scanning tunneling spectroscopy on magnetic field, TAKAHIRO NISHIO, MASANORI ONO, TOYOAKI EGUCHI, The Institute for Solid State Physics, The University of Tokyo, HIDEAKI SAKATA, Department Physics, Tokyo University of Science, YUKIO HASEGAWA, The Institute for Solid State Physics, The University of Tokyo — We performed scanning tunneling microscopy/spectroscopy at low temperature (<2 K) on atomically-flat nano-sized Pb islands formed on the Si(111)-7x7 substrate. The measured tunneling spectra revealed that the superconducting gap does not depend on the sites in a single Pb island but depends on the lateral size of islands. These are consistent qualitatively with the results of a theoretical calculation which includes the fluctuation of superconductivity[1]. We also investigated superconductivity of Pb islands under magnetic fields up to 2.1 T. The superconducting gaps were still observed above the critical magnetic field of bulk Pb. In addition, the obtained spectra showed the decrease in the conductance at zero bias voltage when the island size is small. The conductance decrease can be explained with Gor’kov equations on superconducting spheres whose size is smaller than the coherence length. [1] T. Nishio et al., APL 88, 113115 (2006).

9:24AM N42.00006 STM and LEEM Observations of Pb Growth on W(110), SHIRLEY CHIANG, DONELL HOFFMAN, University of California Davis — We have recently used both scanning tunneling microscopy (STM) and low energy electron microscopy (LEEM) in a combined UHV system to study the growth of Pb on W(110). As seen in previous studies, Stranski-Krastanov growth occurs. STM images show rows of Pb islands. A critical mass of Pb is required before condensation of clusters into stacks occurs at room temperature, while at 200°C the Pb immediately forms distinguishable stacked islands. After the completion of the first monolayer, LEEM observations of this system show the development of 3D Pb crystallites, with the island density depending strongly on temperature. For Pb deposition at a substrate temperature of 200°C, the islands grow together and form larger islands with quasi-hexagonal sides. Annealing the Pb crystallites causes them to merge and reshape while maintaining long-range order. The crystallites melt at the usual Pb melting temperature of 323°C, resulting in small, round, disordered islands. Upon recooling, the islands develop a hexagonal shape. They desorb from the surface at approximately 452°C.

9:36AM N42.00007 STM investigation of quantum size effect on adsorption and reactivity of different gases and alkali metals on thin Pb films¹, ALEXANDER KHAJEETOORIANS, SHENGYONG QIN, MURAT OZER, CHIH-KANG SHIH, The University of Texas at Austin; Department of Physics — Recent work has shown that the Quantum Size Effect (QSE) plays a critical role in the catalytic behavior in reactivity. More specifically, the presence of quantum well states in thin metal systems can have profound effects on surface reactivity. Epitaxial thin Pb films on Si(111) are well known to exhibit pronounced QSE manifested by the phase matching of the Fermi wavelength and the layer thickness, giving rise to bilayer oscillation as well as a re-entrant quantum beats of longer periodicity. Such quantum oscillation phenomena have been observed in preferred film thickness, the location of quantum well states, as well as superconductivity. This work focuses on studies of adsorption and surface reactivity of different gases (hydrogen, oxygen and carbon monoxide) and alkali metal on thin Pb films grown on Si(111) surface.

¹This work is supported by NSF DMR-0606485.

9:48AM N42.00008 Automated Tracking of Nanometer-Scale Feature Evolution Using an STM, RUSSELL LAKE, Clemson University; ADAM DEAN, College of Charleston, NIRU MAHESWARANATHAN, South Carolina Governor’s School for Science and Mathematics, CHAD SOSOLIK, Clemson University — Time-resolved measurements of vacancy pits and adatom islands on monatomic metallic surfaces [e.g. Ag(111)] [1] have provided valuable insight into the underlying atomic diffusion processes that drive dynamics at nanometer length scales. Utilizing our variable temperature scanning tunneling microscope or STM, we are extending this probing method to more complex systems, such as the AuCu and NiAl alloys. To increase the rate of successful data acquisition for these measurements, we have developed automated tracking routines that allow for the continuous monitoring of evolving surface features with minimal operator involvement. Post-acquisition image analysis is further enhanced utilizing feature detection algorithms. Current proof-of-concept results spanning several hours of acquisition time on single crystal metal surfaces are presented. [1] K. Morgenstern et al., Phys. Rev. B 63, 045412 (2001).

10:00AM N42.00009 Chemical Identification in the Cu₃Au (100) Surface Using STM and DFT, RODRIGO B. CAPAZ, UFRJ and Inmetro, Brazil, LUIS G. DIAS, Inmetro, Brazil, ALEXANDRE A. LEITÃO, UFJF and Inmetro, Brazil, RALF-PETER BLUM, HORTST NIEHUS, Humboldt University, Germany, CARLOS A. ACHETE, UFRJ and Inmetro, Brazil — We describe the structure, energetics and electronic structure of the Cu₃Au (100) surface using a combination of scanning tunneling microscopy (STM) and first-principles calculations based on density functional theory (DFT). Our calculations show that the CuAu termination is the one with lower surface energy, in agreement with experiments. The well-known surface atomic rippling is also well reproduced by the calculations. Atomically-resolved STM images show an interesting voltage dependence, showing both types of atoms in the surface unit cell for lower voltages but just one type for higher voltages. Comparisons with theoretically-simulated STM images and cross-sectional electronic density profiles allows for an unambiguous assignment of Au atoms as the one appearing in higher voltage images, thus providing chemical identification at the surface.
Lattice thermal conductivity can be intensive Umklapp scattering originating from low-lying optical phonons.

of 1.4 mdyn/A, indicating that the Ce atoms are bound very weakly with surrounding rigid RuSb using single crystal samples at JRR-3M reactor of JAERI in Tokai. As results, we have found optical phonons associated with large vibration of Ce atoms at 4

origin of their low lattice thermal conductivity. Previous studies suggest that the low thermal conductivity is a consequence of free vibration of rare-earth atoms in the lattice. To improve the performance further, it is important to clarify the factors affecting the thermal conductivity.

Metropolitan Univ. — Filled skutterudite compounds have attracted great attention due to their potential as thermoelectric devices. In particular, their low lattice thermal conductivity is advantageous to achieve high thermoelectric performance. To improve the performance further, it is important to clarify the factors affecting the thermal conductivity. 

In collaboration with Xiaohua Ji, Jian He, Bo Zhang, Nick Gothard, and Paola Alboni, Dept. of Physics, Clemson University. A brief discussion of the synthesis techniques, the characterization techniques and highlights of several systems of materials will be presented.

These nanocomposites give a new level of potential control as a tuning parameter with which to vary the materials' thermoelectric properties. In addition, the transport and magnetic properties of dilute rare-earth-PbSe alloys have been synthesized as nanomaterials using hydrothermal techniques. A

The two-dimensional electron gas in a single graphene sheet exhibits unique properties due to the cone-shaped electron band structure near the Fermi energy. Recently, the growth of a single layer of graphene on SiC(0001) has been demonstrated, opening new possibilities for fabricating large scale graphene-based devices. We have performed scanning tunneling microscopy and spectroscopy of single and bi-layer graphene films on SiC(0001). Atomically resolved topographs and dl/dV maps show clear differences between the single and bi-layer surfaces at different length scales. We have characterized the energy dependence and spatial distribution of the electron local density of states in these single and bi-layer films.

Wednesday, March 7, 2007 8:00AM - 11:00AM — Session N43 FIAP DMP: Focus Session: Physics of Thermoelectric Materials and Phenomena

III Colorado Convention Center 506

8:00AM N43.00001 ABSTRACT WITHDRAWN —

8:12AM N43.00002 Thermoelectric and Thermomagnetic Properties of Nanostructured Lead Chalcogenides. 1

8:24AM N43.00003 Transport and magnetic properties of dilute rare-earth-PbSe alloys. V. JOVIOVIC, S. JOOTTU-THIAGARAJAN, J. WEST, J. P. HEREMANS, The Ohio State University, T. STORY, Z. GOLACKI, W. PASZKOWICZ, V. OSINNYI, Polish Academy of Sciences, Warsaw, Poland — An increase in the density of states is predicted [1] to increase the thermoelectric (TE) figure of merit, and could be induced by doping TE materials with rare-earth elements. This was attempted here: the galvanomagnetic and thermomagnetic properties of dilute alloys of PbSe and Cr, Pr, Nd, Eu, Gd and Yb were measured from 80 to 380K; magnetic susceptibilities were measured from 4 to 120K. The density of states effective mass, the relaxation time, and the carrier density and mobility are calculated from measurements of the electrical conductivity and the Hall, Seebeck and transverse Nernst-Enthtssen coefficients. The Eu, Gd, Nd and Yb-alloyed samples are paramagnetic; the concentrations of rare-earth atoms are determined from fitting a Curie-Weiss law. The magnetic behavior of the Ce and Pr-alloyed samples is different. Ce, Pr, Nd, Gd and Yb act as donors with efficiencies that will be reported. alloying with divalent Eu does not affect carrier density but increases the energy gap. This work suggests that the f orbitals preserve their atomic-like localized character and exhibit only weak sp-f hybridization. 1 G. D. Mahan and J. O. Sofo, Proc. Natl. Acad. Sci. USA 93 7436 (1996).

8:36AM N43.00004 Synthesis & Properties of Nano-Composite Thermoelectric Materials. TERRY TRITT, Dept. of Physics, Clemson University — PbTe nanocrystals have been grown in our labs by chemical vapor deposition. These materials grow in size selective regions exhibiting very high yield and have size distributions of around 100 nm to 1000 nm. These nano-materials are incorporated into a bulk matrix, making a composite material in hopes of achieving a higher thermoelectric performance due to the increased phonon scattering that the nano-materials are expected to exhibit, as well as potential for enhancement of their Seebeck coefficient. Some of the advantages as well as the challenges will be discussed. These nanocomposites give a new level of potential control as a tuning parameter with which to vary the materials' thermoelectric properties. In addition, Bi2Te3, another state of the art thermoelectric material and skutterudites (CoSb3) have been synthesized as nanomaterials using hydrothermal techniques. A brief discussion of the synthesis techniques, the characterization techniques and highlights of several systems of materials will be presented.

In collaboration with Xiaohua Ji, Jian He, Bo Zhang, Nick Gothard, and Paola Alboni, Dept. of Physics, Clemson University. 3

Acknowledgment DOE/EPSCoR Grant (DE-FG02-04ER-46139)

9:12AM N43.00005 Neutron scattering study of phonon dynamics on cage compounds. C.H. LEE, AIST Jpn, H. HOSHIYAMA, ISSP, I. HASE, AIST, H. SUGAWARA, Tokushima Univ., M.A. AVILA, T. TAKABATAKE, Hiroshima Univ., H. SATO, Tokyo Metropolitan Univ. — Filled skutterudite compounds have attracted great attention due to their potential as thermoelectric devices. In particular, their low lattice thermal conductivity is advantageous to achieve high thermoelectric performance. To improve the performance further, it is important to clarify the origin of the low lattice thermal conductivity. Previous studies suggest that the low thermal conductivity is a consequence of free vibration of rare-earth atoms in large lattice cages, which is so called rattling effect. To confirm the hypothesis, we have studied phonon dynamics of CeRu2Sb12 by neutron scattering using single crystal samples at JRR-3M reactor of JAERI in Tokai. As results, we have found optical phonons associated with large vibration of Ce atoms at relatively low energy of E=6meV, which show an anticrossing with acoustic phonons. According to the analysis based on a Born-von K'arm'an force model, the longitudinal force constants of the nearest Ce-Sb and Ce-Ru are both estimated to be 0.025 mdyn/A, while that of the nearest Ru-Sb shows a large value of 1.4 mdyn/A, indicating that the Ce atoms are bound very weakly with surrounding rigid RuSb12-octahedron cages. We will discuss that the origin of the low lattice thermal conductivity can be intensive Umklapp scattering originating from low-lying optical phonons.
9:24AM N43.00006 Superconductivity of Ba8Si46-xGax clathrates. YANG LI, Department of General Engineering, University of Puerto Rico at Mayaguez, PR 00681, USA, RUHONG ZHANG, NING CHEN, XINGQIAO MA, GUOHUI CAO, Department of Physics, University of Science and Technology Beijing, 100083, China, Z.P. LUO, C.R. HU, JOSEPH H. ROSS, JR., Department of Physics, Texas A&M University, College Station, TX 77843 — We have presented a combined experimental and theoretical study of the effect of Gallium substitution on the superconductivity of the type I clathrate Ba8Si46-xGax. In Ga-doped clathrates, the Ga state is found to be strongly hybridized with the cage conduction-band state. Ga substitution results in a shift toward to a lower energy, a decrease of density of states at Fermi level, a lowering of the carrier concentration and a breakage of integrity of the sp3 hybridized networks. These play key roles in the suppression of superconductivity. For Ba8Si40Ga6, the onset of the superconducting transition occurs at Tc=3.3 K. The magnetic investigation of the superconducting state shows that Ba8Si40Ga6 is a type II superconductor. The critical magnetic fields were measured to be Hc1=35 Oe and Hc2=8.5 kOe. Our estimate of the electron-phonon coupling reveals that Ba8Si40Ga6 is a moderate phonon-mediated BCS superconductor.

9:36AM N43.00007 Thermoelectric Properties of RE3Ru4Ge13 compounds (RE = Y, Dy, Ho, Lu). D. MORELLI, Michigan State University, H. KONG, X. SHI, C. UHER, University of Michigan — Rare earth based compounds have been suggested as ideal thermoelectric materials due to the potential existence of sharp features in their electron density of states. One such series of compounds is of the form RE3Ru4Ge13. These materials crystallize in the cubic structure Pm3n and are known to exhibit a variety of interesting properties, including magnetic ordering, superconductivity, and anomalous semiconductor-like resistivity. These compounds can be considered as variants of the cubic structure compound RE4Ru3Ge12 (RE=Eu, Ru, RE=Er, Ru, Ge2) in which one RE atom is replaced by a germanium atom. This “extra” Ge atom can reside on either the Ge or RE site, and the site disorder combined with the complex unit cell of these compounds suggests inherent low lattice thermal conductivity. In order to survey the potential of these materials as thermoelectrics we have synthesized several members of this family. Results on Seebeck coefficient, resistivity, Hall coefficient, and thermal conductivity as a function of temperature will be reported.

9:48AM N43.00008 The thermoelectric properties of Bi nanowires. Role of quantum size and surface effects. TITO HUBER, Howard University, 500 College St. N.W., Washington DC 20059, ALBINA NIKOLAEVA, DMITRI GITSU, LEONID KONGPKO, Institute of Applied Physics, Academy of Sciences, Moldova, MICHAEL GRAF, Department of Physics, Boston College, Chestnut Hill, MA 02467. — Because of the increased density of states arising from one-dimensional confinement, it is anticipated that bismuth quantum wires will exhibit superior thermoelectric properties. Recently, angle-resolved photoemission spectroscopy (ARPES) studies have shown that Bi supports surface states that have not been considered in current models of quantum confinement. Studies of the Fermi surface, employing the Shubnikov-de Haas (SdH) method, in arrays of 30- to 80-nm bismuth nanowires partially corroborates ARPES findings. Assuming diffusive conditions, the impact of the excess surface carriers on the thermopower is to effectively make it smaller than that of bulk Bi, in agreement with measurements reported in the literature. We will report the result of experiments designed to decrease the concentration of surface carriers.

1Supported by National Science Foundation and Army Research Office

10:00AM N43.00009 Thermoelectric properties of SiGe nanoparticle composites. MING TANG, HOHYUN LEE, ASEGUN HENRY, Massachusetts Institute of Technology, RONGGUI YANG, University of Colorado at Boulder, DEZHI WANG, Boston College, JEAN-PIERRE FLEURIAL, PAWAN GOGNA, Jet Propulsion Laboratory, GANG CHEN, Massachusetts Institute of Technology, ZIFENG REN, Boston College, MILDRED DRESSHELHAN, Massachusetts Institute of Technology — Prior theoretical and experimental proof of principle studies on quantum well superlattices and quantum wire samples have now evolved into studies on bulk samples containing nanostructured constituents prepared by chemical or physical approaches. We have shown that nanostructural composites exhibit nanostructures and properties that show great promise for thermoelectric applications, thus bringing together low-dimensional and bulk materials for thermoelectric applications. We demonstrate that we can achieve (1) a simultaneous increase in the power factor and a decrease in the thermal conductivity in the same nanocomposite sample and (2) lower values of the thermal conductivity in these nanocomposites as compared to alloy samples of the same chemical composition. The outlook for future research directions for nanocomposite thermoelectric materials is also discussed.

1This work is funded by NASA Contract #NASS-03108.

10:12AM N43.00010 Synthesis and Characterization of Nanocomposite Chalcogenides. JOSHUA MARTIN, Department of Physics, University of South Florida, Tampa, FL 33620 USA, W. ZHANG, L. CHEN, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, China, G.S. NOLAS, Department of Physics, University of South Florida, Tampa, FL 33620 USA, DEPARTMENT OF PHYSICS, UNIVERSITY OF SOUTH FLORIDA, TAMPA, FL 33620 USA TEAM, SHANGHAI INSTITUTE OF CERAMICS, CHINESE ACADEMY OF SCIENCES, SHANGHAI 200050, CHINA COLLABORATION — Recent results on the thermoelectric properties of superlattices and nano-scale materials have energized the search for high-performance thermoelectric materials. Thermoelectric technology requires materials in large quantities therefore new approaches are needed to incorporate nano-scale enhancement into bulk materials. We present a technique to synthesize dense bulk nanocomposites reproducibly, and investigate their structural and transport properties. Transport properties demonstrate a strong dependence on porosity, highlighting the necessity of dense nanocomposites for thermoelectric applications.

10:24AM N43.00011 Time-Resolved Diffraction Studies of Nanoscale Thermal Transport. MATT HIGHLAND, BRYAN GUNDERM, YEE KAN KOH, VICTOR ELARDE, JAMES J. COLEMAN, DAVID G. CAILL, University of Illinois Urbana/Campaign, DON WALKO, ERIC LANDAIH, Argonne National Laboratory Advanced Photon Source — One of the major considerations in fabricating devices on ever smaller length scales is thermal management in nanometer sized structures. Studying thermal transport requires a temperature measurement accurate on short time scales and sensitive to temperature changes in nanoscale structures. Time Resolved X-ray Diffraction (TRXD) utilizes 100ps x-ray pulses as a probe of lattice expansion and ultrafast laser pulses as a pump to probe the temperature of optically excited materials. Thermal expansion due to laser heating can therefore be used to study thermal transport in thin films. Reported here are (TRXD) measurements of the temperature rise in (lnAs)x(GaAs)y thin films due to laser heating. These results are compared with continuum model predictions of temperature rise based on film parameters measured independently using Time Domain Reflectance. This comparison shows a continuum model is inadequate in predicting the thermal behavior these films on short time scales and is indicative of complex transport phenomenon.
The survey have been completed, and the results and methodology will be presented. Moderate or high values does not exist. In an effort to expedite research efforts in this field, we have initiated a project to develop a Seebeck coefficient, or conductivity, and Seebeck coefficient. While standard materials exist or have existed for the first two properties, a Seebeck coefficient standard material with moderate or high values does not exist. In an effort to expedite research efforts in this field, we have initiated a project to develop a Seebeck coefficient, or thermopower, standard reference material. To this end, we have conducted a round-robin measurement survey of candidate standard materials. Both rounds of the survey have been completed, and the results and methodology will be presented.

**Wednesday, March 7, 2007 8:00AM - 10:36AM**

Session N44 DMP: Focus Session: Optical Properties of Nanowires and Nanocrystals Colorado Convention Center 507

10:36AM N43.00012 Thermoelectric Properties of Heterostructure InAs/InP Nanowires. Eric Hoffmann, University of Oregon, Ann Persson, University of Oregon/Lund University, Henrik Nilsson, Linus Fröberg, Lars Samuelson, Lund University, Heiner Linke, University of Oregon — InAs nanowires with an embedded quantum dot defined by an InP double-barrier structure offer quantum confinement in all three spatial directions. Using a global gate, the Fermi energy can be tuned relative to the dot’s density of states. Furthermore, at temperatures below ~10 K, phonon states freeze out, decoupling phonons and electrons, and electron temperatures can be controlled independently of the lattice temperatures. Due to this control, nanowires at low temperatures lend themselves to detailed investigations of the dependence of thermoelectric effects on a strongly modulated density of states. This is of interest, because such systems have been predicted to be able to convert thermal energy to electrical energy at very high efficiency. We report on experiments where a temperature gradient in the electron gas is created along a single nanowire by heating the metallic lead at one end of the nanowire using an ac heating current. The resulting temperature gradient creates a thermovoltage across the nanowire whose sign and magnitude can be tuned by adjusting the Fermi energy relative to the discrete energy levels in the quantum dot. We find that the thermovoltage depends nonlinearly on the temperature differential at surprisingly small temperature gradients.

10:48AM N43.00013 Round-robin measurement survey for Seebeck coefficient standard reference material. Nathan Lowhorn, Winnie Wong-ng, Makoto Otani, Martin Green, National Institute of Standards and Technology, Thanh Tran, Naval Surface Warfare Center — Full characterization of a thermoelectric material requires measurement of the electrical resistivity, thermal conductivity, and Seebeck coefficient. While standard materials exist or have existed for the first two properties, a Seebeck coefficient standard material with moderate or high values does not exist. In an effort to expedite research efforts in this field, we have initiated a project to develop a Seebeck coefficient, or thermopower, standard reference material. To this end, we have conducted a round-robin measurement survey of candidate standard materials. Both rounds of the survey have been completed, and the results and methodology will be presented.

**8:00AM N44.00001 Electronic and optical properties of single-walled GaN nanotubes from first principles.** Sohrab Ismail-beigi, Yale University — There is current experimental interest in fabricating GaN nanotubes for possible optoelectronics/photoluminescence applications. To date, *ab initio* studies of these potentially interesting systems have used ground-state density functional theory which has well-known shortcomings when used to predict electronic excitations. We report on our *ab initio* predictions of the electronic and optical properties of single-walled GaN nanotubes using electronic Green's functions within the GW-Bethe Salpeter Equation formalism. We present results the nanotube band structures, optical spectra, excitonic states, and likely luminescence properties.

**8:12AM N44.00002 Optical Second-Harmonic Generation from Single GaN Nanowires.** J.P. Long, B.S. Simpkins, D.J. Rowenhurst, P.E. Persson, Naval Research Laboratory, Washington DC 20375 — The nonlinear optical response of nanostructured materials is of interest because of the need for active elements in nanophotonic applications, and because the nonlinear response can provide information about the nanostructure itself. Here we report measurements of second-harmonic generation (SHG) from individual GaN nanowires (NWs) based on far-field optical microscopy. By correlating the polarization behavior of the SHG signal from each NW with its orientation as determined with electron backscattered diffraction, we show that far-field methods can provide a flexible approach for distinguishing the crystallographic orientations of wurtzite NWs lying on a substrate. Analysis is based on the quasi-static approximation, which assumes that a NW's transverse dimension (75 nm) is less than the relevant wavelengths and thus permits treating the optical electric-fields as spatially uniform. This approach proves sufficient to explain the main SHG polarization features of these NWs, once one accounts for internal depolarization effects for both the excitation and SH electric fields, and for the collection-aperture of the microscope objective.

1 Funded by ONR.

**8:24AM N44.00003 Non-Equilibrium Exciton Spin Dynamics in Resonantly Pumped Single Core-Shell GaAs-AlGaAs Nanowires.** Thang B. Hoang, L.V. TitoVA, H.E. Jackson, L.M. Smith, University of Cincinnati, J.M. Yarrison-Rice, Miami University, A.O. Govorov, Ohio University, Y. Kim, H.J. Joyce, H.H. Tan, C. Jagadish, Australian National University — We use spatially-resolved photoluminescence (PL) imaging in combination with polarized resonant excitation to investigate the non-equilibrium exciton spin states in single core-shell GaAs-AlGaAs nanowires (~40 nm core diameter) at low temperature. The large dielectric mismatch between the nanowire and the vacuum results in a strong polarization of excitonic dipoles in the nanowire. This leads to strong polarization of both exciton excitation and emission along the nanowire. Resonant excitation shows two resonances at 1-LO and 2-LO phonons of GaAs and a third resonance likely from electronic states of the AlGaAs. More interestingly, we observe that the polarization of the PL emission is strongly enhanced as the excitation energy comes closer to resonance with the exciton emission. This strong polarization enhancement indicates that resonant excitation creates non-equilibrium exciton spin distributions near resonance. Rate equation modeling allows us to estimate the spin relaxation times which range from ~5ps at high energies to ~50ps at energies close to resonance. Financial support for this work was provided by the University of Cincinnati, Ohio University and the Australian Research Council.

**8:36AM N44.00004 Photoluminescence dynamics of single InP nanowires.** L.V. Titova, A. Mishra, Thang B. Hoang, H.E. Jackson, L.M. Smith, University of Cincinnati, J.M. Yarrison-Rice, Miami University, H.J. Joyce, Y. Kim, Q. Gao, H.H. Tan, C. Jagadish, Australian National University — We use time-resolved photoluminescence (PL) spectroscopy to study exciton dynamics in single InP nanowires prepared by catalyst-assisted vapor-liquid-solid growth. In contrast to other III-V materials like GaAs, InP has a lower surface recombination velocity, which should result in longer excitonic lifetimes and higher quantum efficiencies. Indeed, the InP nanowires exhibit emission lifetimes ranging from 80 ps to 2 ns compared to <80 ps lifetimes observed for GaAs-AlGaAs nanowires. The large variation in the lifetimes from nanowire to nanowire may be the result of structural inhomogeneities and defects that act as nonradiative recombination centers, thus limiting the excitonic lifetimes. In addition, we have observed changes in the recombination dynamics for single InP nanowires as a function of energy. On the high energy side of the PL peak, the recombination rate is rapid (~50 ps), while on the low energy side it is significantly slower (up to 1 ns) due to the spectral diffusion of carriers. Preliminary polarization measurements show rapid depolarization of the PL during the ~75 ps emission risetime due to spin scattering of excitons. Financial support for this work was provided by the University of Cincinnati and the Australian Research Council.
The DDA model results are shown to depend on the nanowire diameter/length and the thickness of amorphous SiO\textsubscript{2} shell.

The experimental absorption spectrum will be explained on the basis of dielectric function calculations carried out in the discrete dipole approximation (DDA).

Si-NCs treated by CF\textsubscript{4} significantly, relatively high quantum yields of short-wavelength light emission from Si-NCs are obtained in spite of oxidation. It is interesting to note that light in the short-wavelength region from yellow to blue. We find that a self-limited oxidation process blueshifts the light emission until saturation is reached.

Photoluminescence spectra on 3 sets of Si nanowires with most probable diameter 3.5 nm, 5.5 nm and 9 nm are presented. In the optical absorption, apart from the direct gap absorption at E\textsubscript{g} of 3.4 eV and E\textsubscript{g} = 2.5 eV. Interestingly, these lower energy features are not expected on the basis of the bulk dielectric function of Si. They are observed experimentally to increase in intensity with decreasing nanowire diameter. It is obvious that these features model calculations, which passivates them with carbon and fluorine. After the two-stage process Si-NCs emit very high density of defects such as Si dangling bonds at the Si-NC/oxide interface. Therefore, the PL efficiency is extremely low for short-wavelength light emitting Si-NCs. Yellow or green photoluminescence (PL) has been observed from initially oxidized red light emitting Si-NCs after HF vapour etching and atmospheric oxidation.

An electrically pumped Si laser would present a breakthrough for optoelectronic integration that may enable optical interconnect to make computers faster.

Minneapolis 55455 — Si is the material of choice for modern microelectronics but, as an indirect-bandgap semiconductor, it is not an efficient light emitter. Computer Engineering, University of Minnesota, Minneapolis 55455, UWE KORTSHAGEN, Department of Mechanical Engineering, University of Minnesota, Minneapolis 55455 — Diluted Magnetic Semiconductor (DMS) have attracted a lot of attention in the field of Spintronics. Here, we report on our progress to grow DMS Zn\textsubscript{1-x}MnxS \((0 \leq x \leq 0.6)\) nanowires using the vapor-solid growth mechanism and CVD source techniques based on sublimation of ZnS and MnCl\textsubscript{2} powder. Ar/H\textsubscript{2} carrier gas was passed over ZnS and MnCl\textsubscript{2} maintained at specific temperatures to control the Zn/Mn ratio in the stream. The Zn/Mn concentration also is found to determine the structure, i.e., wurzite vs zinc blende. H. WU, HUMBERTO GUTIERREZ, PETER EKLUND, Department of Physics, Pennsylvania State University — Diluted Magnetic Semiconductor (DMS) have attracted a lot of attention in the field of Spintronics. Here, we report on our progress to grow DMS Zn\textsubscript{1-x}MnxS \((0 \leq x \leq 0.6)\) nanowires using the vapor-solid growth mechanism and CVD source techniques based on sublimation of ZnS and MnCl\textsubscript{2} powder. Ar/H\textsubscript{2} carrier gas was passed over ZnS and MnCl\textsubscript{2} maintained at specific temperatures to control the Zn/Mn ratio in the stream. The Zn/Mn concentration also is found to determine the structure, i.e., wurzite vs zinc blende. H. WU, HUMBERTO GUTIERREZ, PETER EKLUND, Department of Physics, Pennsylvania State University — The electronic and magnetic properties of semiconductor nanowires require new measurement techniques. In this paper, we present a stroboscopic imaging technique using an optical microscope. This technique enables the measurement of the band edge non-radiative states of Si-NCs. The signal-to-noise ratio of the image may be determined with a precision given by the signal-to-noise ratio rather than by the optical resolution. We demonstrate an accuracy below 1 nm, more than two orders of magnitude better than the diffraction limit. Temporal information is obtained stroboscopically using a pulsed LED as a light source. The time-resolution is given by the width of the light pulses which in our experiments is below 100 ns. The nanowires are electrostatically bent by applying a voltage between the nanowire and a nearby W-needle. By applying voltage pulses we induce damped oscillations and by applying a sinus voltage we drive the nanowire at varying frequency. In both cases we get resonance frequencies of a few MHz for nanowires about 100 nm in diameter and 5 \(\mu\)m long.

Optical absorption in small diameter Si nanowires \(KOFI ADU, GUGANG CHEN, HUMBERTO GUTIERREZ, PETER EKLUND, Department of Physics, Pennsylvania State University, University Park, PA 16802, U.S.A. — Optical absorption spectra on 3 sets of Si nanowires with most probable diameter 3.5 nm, 5.5 nm and 9 nm are presented. In the optical absorption, apart from the direct gap absorption at E\textsubscript{g} \(\approx 3.4\) eV and E\textsubscript{g} \(\approx 4.2\) eV, we observed two additional strong absorption bands near 1.5 eV and \(\approx 2.5\) eV. Interestingly, these lower energy features are not expected on the basis of the bulk dielectric function of Si. They are observed experimentally to increase in intensity with decreasing nanowire diameter. It is obvious that these features model calculations, which passivates them with carbon and fluorine. After the two-stage process Si-NCs emit very high density of defects such as Si dangling bonds at the Si-NC/oxide interface. Therefore, the PL efficiency is extremely low for short-wavelength light emitting Si-NCs. Yellow or green photoluminescence (PL) has been observed from initially oxidized red light emitting Si-NCs after HF vapour etching and atmospheric oxidation.

The DDA model results are shown to depend on the nanowire diameter/length and the thickness of amorphous SiO\textsubscript{2} shell.

Low temperature photoluminescence of single InP nanowires \(XIAODONG WU, HUMBERTO GUTIERREZ, PETER EKLUND, Department of Physics, Pennsylvania State University — Low temperature photoluminescence of single InP nanowires. In the optical absorption, apart from the direct gap absorption at E\textsubscript{g} \(\approx 3.4\) eV and E\textsubscript{g} \(\approx 4.2\) eV, we observed two additional strong absorption bands near 1.5 eV and \(\approx 2.5\) eV. Interestingly, these lower energy features are not expected on the basis of the bulk dielectric function of Si. They are observed experimentally to increase in intensity with decreasing nanowire diameter. It is obvious that these features model calculations, which passivates them with carbon and fluorine. After the two-stage process Si-NCs emit very high density of defects such as Si dangling bonds at the Si-NC/oxide interface. Therefore, the PL efficiency is extremely low for short-wavelength light emitting Si-NCs. Yellow or green photoluminescence (PL) has been observed from initially oxidized red light emitting Si-NCs after HF vapour etching and atmospheric oxidation.

The DDA model results are shown to depend on the nanowire diameter/length and the thickness of amorphous SiO\textsubscript{2} shell.

8:48 AM N44.00005 Low temperature photoluminescence of single InP nanowires — A. MISHRA, D. SHEREEN, THANG B. HOANG, L.V. TITTOVA, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J.M. YARRISON-RICE, Miami University, H.J. JOYCE, Y. KIM, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University — We investigate low-temperature optical emission properties of a number of single InP nanowires prepared by catalyst-assisted vapor-liquid-solid growth. Photoluminescence (PL) spectra of the nanowires display a broad (full width at half maximum of \(27 \pm 3\) meV) peak centered at 1.414 ± 0.008 eV, often accompanied by a broader lower energy shoulder at \(\sim 1.378 \pm 0.008\) eV. The variability in energy of the main peak, which may correspond to bandgap emission, may be explained by structural and compositional variations and non-uniformities of the nanowires. The measured lower energy shoulder position is not clear but is likely related to the defect states. We find the band gap narrowing, i.e., the DDA model results are shown to depend on the nanowire diameter/length and the thickness of amorphous SiO\textsubscript{2} shell.
10:00AM N44.00011 Dynamical and Optical Properties of Si and Ge Nanocrystals. KELLY KNUTSEN, MATT BEARD, P.R. YU, QING SONG, WYATT METZGER, ART NOZIK, RANDY ELLINGSON, National Renewable Energy Lab — Si nanocrystals exhibit the unusual property of having a high photoluminescence quantum yield as well as a long first exciton lifetime. This implies that the decay rates for the non-radiative channels have decreased compared to the bulk. We explore this phenomenon by first characterizing the optical properties of the Si nanocrystals by measuring their linear absorption and photoluminescence spectra as a function of nanocrystal size, which show an expected shift to the blue for the transition onset with decreased particle size. The nanoparticles exhibit indirect transition characteristics, and emit roughly 1eV to the red of the absorption onset. We also employ time-resolved photoluminescence (TRPL) and transient absorption (TA) spectroscopy to investigate the Auger dynamics of the single and bieexcitons. Initial results for 9nm Si nanoparticles show that the bieclexiton lifetime is roughly 200 ps and the single exciton lifetime is greater than 200 microseconds. The size dependence on the single and bieclexiton lifetimes, as well as the potential presence of multiple exciton generation (MEG) in these materials will be presented. Initial optical studies of Ge nanocrystal charge carrier dynamics will also be presented.

10:12AM N44.00012 Visible light absorption and photodarkening in Te-modified TiO2 nanocrystals. STEVEN PHILLIPS, IAN JAMES, BRETT HESS, Brigham Young University — Applications of titanium dioxide nanocrystals in solar cells and solar photocatalysis are limited by the lack of visible light absorption. We have created TiO2 nanocrystals modified by tellurium, which causes absorption in the visible. In TiO2:Te nanocrystals annealed between 300 and 600 C, light exposure quickly causes the visible absorption to increase until the sample is reddish-brown. The presence of Te stabilizes the anatase structure, while the rutile phase is found in undoped nanocrystals. We discuss possible mechanisms for the photodarkening, and explore whether this visible absorption is useful in photocatalysis.

10:24AM N44.00013 Density Matrix Approach for Valence Band Optical Properties1, M.P. PRANGE2, J.I. REHR, University of Washington — We present an extension of the ab initio real-space multiple-scattering (RSMS) theory currently used for core-level spectra (e.g. EELS, XAS and NRIXS) to calculations of the valence band optical response. The method is based on RSMS calculations of the occupied and unoccupied density matrices and transition matrix elements between the two resulting in an efficient way to calculate various optical constants in aperiodic materials. In contrast to bandstructure or basis-set methods, the calculation can be applied to a large class of materials, including both insulators and metals up to the nanoscale. By combining the method with the RSMS approach for core level response, we obtain an approach applicable for spectra from the far IR to x-rays. Results are compared with experiment and with other theoretical techniques. Possible extensions are also discussed.

Wednesday, March 7, 2007 11:15AM - 2:15PM — Session P8 DMP: Focus Session: Novel Superconductors:Miscellaneous Materials Colorado Convention Center Korbel 1C

11:15AM P8.00001 Recent progress in applications of the superconducting density functional theory1, SANDRO MASSIDDA, Dipartimento di Fisica, University of Cagliari, Italy — One of the great challenges of condensed-matter theory is the prediction of material specific properties of superconductors (SC) such as the critical temperature Tc or the gap at zero temperature. Recently, based on a seminal work by Oliveira, Gross and Kohn(1), an extension of density functional theory to the superconducting state (SCDFT) was introduced and applied to elemental superconductors (2). Later work showed how the method is able to describe the properties of real materials ranging from weak to strong coupling. Unique feature of the method is the ab-initio inclusion of the Coulomb interaction which, recently combined with a fully anisotropic treatment of the electron-phonon coupling, allows for a detailed description of the most important material specific properties, including the relevance of multiple gaps, in good agreement with the available experiments.

The discovery of novel electron-phonon SC provided new challenges to the method. We will report on the most recent applications, including MgB2, alkali metals under pressure, Ca intercalated graphite and other new and traditional SC. The subtle interplay between e-ph mediated attraction and Coulomb repulsion, normally hidden by the use of the pseudopotential µ∗, will show its material-specific importance in the resulting Tc. (1) L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. 60, 2430 (1988) (2) Marques et al., Phys Rev. B 72, 024545 (2005); M. Lueders et al., ibid 024546 (2005)

1I acknowledge financial support by MIUR under the projects PRIN2004022024 and PON-CyberSar.

11:51AM P8.00002 First-Principles Investigation of Superconductivity in Transition Metal Carbides1, JESSE NOFFSINGER, FELICIANO GIUSTINO, STEVEN G. LOUIE, MARVIN L. COHEN, UC Berkeley, Lawrence Berkeley National Laboratory — We investigate the origin of superconductivity in the transition metal carbides TaC and HfC by a first-principles approach. The electronic structure is described within density functional theory in the local density approximation, and the lattice dynamical properties are determined through density functional perturbation theory. We calculate the average electron-phonon coupling strength through the isotropic approximation to the Migdal-Eliashberg theory, and the relative transition temperature through the McMillan formula. The calculated transition temperatures are found to be in excellent agreement with experiment. The relatively high transition temperature of TaC (10.3 K) is associated with a Kohn anomaly in the phonon dispersions, and arises from significant Fermi surface nesting. In contrast, the absence of nesting in HfC results in a limited phase-space availability for electron-phonon scattering. Correspondingly, HfC exhibits a negligible transition temperature (~0.1 K).

1This work was supported by National Science Foundation Grant No. DMR04-39768, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and NPACI

12:03PM P8.00003 Strong Electron-Phonon Coupling in Elemental Metals Under Pressure. ZHIPING YIN, WARREN PICKETT, Physics Department, UC Davis — The superconductivity of yttrium with Tc=20K at 115 GPa has been confirmed by strong electron-phonon coupling obtained using linear response methods. The increase of Tc under pressure mainly comes from the increasing strong coupling to the transverse modes at all high-symmetry zone boundary points X, K, and L. Evaluation of the electron-phonon spectral function shows a very strong increase with pressure of coupling strength in the 2-8 meV range, but with an accompanying steady increase in the 8-20 meV range. The superconductivity of Ca under pressure, however, is a challenge. While other elemental superconductors are usually close-packed, Ca is simple cubic (SC) at pressure between 30 GPa and 109 GPa, and its Tc increases significantly in this pressure range, and goes to 23 K at 109 GPa (25 K at 161 GPa), making Ca the highest Tc superconductor among elements. From linear response calculations we find the harmonic frequencies are unstable over a large portion of the zone for a wide range of pressure in the SC phase. We present calculational results and discuss possibilities, which include the likely stabilization of the SC structure by large anharmonic contributions to the lattice dynamics.
12:15PM P8.00004 Calculations of Superconducting Properties in Yttrium and Calcium under High Pressure1. DIMITRIOS PAPACONSTANTOPOULOS, LEI SHI, Department of Computational and Data Sciences, George Mason University, Fairfax VA, MICHAEL MEHL, Center for Computational Materials Science, Naval Research Laboratory, Washington DC — We have used first-principles electronic structure calculations to generate the bulk modulus as a function of volume as well as the densities of states and scattering phase shifts at the Fermi level. These quantities were used in conjunction with the rigid-muffin-tin theory of Gasparrini and Györffy and the McMillan theory to determine the electron-phonon coupling and the superconducting transition temperature for Yttrium and Calcium under high pressures. Our results provide a good interpretation of the measured increase of \(T_c\) in these metals.

1Supported by the Office of Naval Research.

12:27PM P8.00005 Assessment of the importance of correlation effects in Li\(_x\)NbO\(_2\). K.-W. LEE, R. T. SCALETTAR, W. E. PICKETT, Univ. of California, Davis, J. KUNES, Univ. of Augsburg — About 15 years ago Gesellbract et al. reported superconductivity with \(T_c=5K\) for \(x \approx 0.5\) in Li\(_x\)NbO\(_2\). The critical temperature does not show significant change in the range 0.45 < \(x\) < 0.8. The electronic structure is based on a strongly two-dimensional triangular Nb lattice, and the superconducting phase is hole-doped from \(x=1\) band isolated within a wide gap, giving a single-band triangular lattice system. The single band has a band width \(W=1.7\) eV and hopping parameters \(t_1=64, t_2=100, t_3=33\) (in units of meV), showing second nearest neighbor hopping to be dominant. To study possible correlation effects, we apply DMFT using on-site Coulomb repulsion \(U=0-4\) eV and obtain the spectrum with MaxEnt. Even \(U=1\) eV is found to cause substantial change in the spectrum, suggesting the importance of correlation effects in Li\(_x\)NbO\(_2\).

12:39PM P8.00006 Nearly-free electron superconductor Ag\(_x\)Pb\(_2\)O\(_4\). SHINGO YONEZAWA, Department of Physics, Graduate School of Science, Kyoto University, Japan, MIKE SUTHERLAND, PETER D. A. MANN, CHRISTOPH BERGMANN, Cavendish Laboratory, University of Cambridge, United Kingdom, YOSHITERU MAENO, Department of Physics, Graduate School of Science, Kyoto University, Japan — Superconductivity in the silver lead oxide Ag\(_x\)Pb\(_2\)O\(_4\) has been discovered below 52 mK [1,2]. Although its \(T_c\) is one of the lowest among the known oxide superconductors, this oxide is interesting from the viewpoint that it is the first superconductor with a nearly-free-electron Fermi surface. This fact is revealed by our quantum oscillation study [3] as well as recent band-calculation studies, which concluded that the system possesses one near-spherical Fermi surface with a small electron–mass enhancement. We will present its type-I superconducting properties, as well as the properties of the normal state where the resistivity varies nearly as \(T^2\) up to room temperature [1].


1The authors acknowledge the support of the Grant-in-Aid “Invention of Anomalous Quantum Materials” from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

12:51PM P8.00007 Electron-phonon interaction in the polymeric superconductor, polysulfur nitride, (SN)\(_x\). PAUL M. GRANT, W2AGZ Technologies — In early 1975, superconductivity at temperatures between 0.3 – 0.4 K was discovered in the inorganic polymer, polysulfur nitride, (SN)\(_x\). The compound itself was originally synthesized in the first decade of the 20th century, but its transport properties were largely undetermined until their investigation was sparked by the emergence of the low dimensional layered organic charge transfer salts in the decade of the 1980s. The issue of why the transition temperature of (SN)\(_x\) is so low has not been adequately addressed computationally, especially in view of the realization of superconductivity at nearly 40 K in magnesium diboride, MgB\(_2\), in 2001, a compound whose electronic structure is remarkably similar to (SN)\(_x\), in that both are two-band, hole-electron semimetals with low-dimensional Fermi surface topologies. In this talk, we report our results on the calculation of the electron-phonon dispersion relation, \(\alpha^2 F(\omega)\), for (SN)\(_x\) obtained from the application of recently available DFT algorithms capable of accurately treating screening of electron-phonon interactions in metals.

1:03PM P8.00008 Microscopic theories for Cubic and Tetrahedral Superconductors1. SHANTANU MUKHERJEE, DANIEL AGTERBERG, University of Wisconsin-Milwaukee — We will examine the weak coupling theory for the unconventional superconducting states of cubic or tetrahedral superconductors for arbitrary order parameters and Fermi surfaces in zero applied magnetic fields. We will also look at multiple transitions where a higher symmetry is weakly broken to account for them. We will then perform a weak coupling theory where two representations of the symmetry group have accidentally nearly degenerate transition temperatures.

1This work was supported by National Science Foundation Grant No. DMR-0381665.

1:15PM P8.00009 Density of states, specific heat and nuclear spin-lattice relaxation rate in Pr\(_{12}\)Sb\(_{12}\). TAYSEER ABU ALRUB, STEPHANIE CURNOE, Department of Physics and Physical Oceanography, Memorial University of Newfoundland — We present a theoretical study of the density of states, specific heat and nuclear spin-relaxation rate in the unconventional superconductor Pr\(_{12}\)Sb\(_{12}\). In this material, superconductivity is best described by a three component order parameter in the triplet channel. Instead of nodes, deep dips appear in the gap. A ~10% discrepancy is found at intermediate temperatures. This seems likely to be due to multiband superconductivity in this compound, recently found from thermal conductivity measurements. A sufficiently large difference between gaps would render the field distribution in the vortex controlled exclusively by the larger gap band, whereas all bands would participate in zero field.

1Supported by NSF Grants 0422674 (Riverside), 0203524 (Los Angeles), 0335173 (San Diego), by Canadian NSERC and CIAR (Burnaby), and by DOE DE-FG02-04ER46105 (San Diego).
1:39PM P8.00011 Fully gapped s-wave superconductivity in KOs$_2$O$_3$. I. BONALDE, R. RIBEIRO, W. BRAMER-ESCAMILLA, Centro de Fisica, IVIC, Apartado 21874, Caracas 1020-A, Venezuela, Z. HIROI, Y. YAMAURA, Institute for Solid State Physics, University of Tokio, Kashiwa, Chiba 277-8581, Japan — The discovery of superconductivity in the β-pyrochlore oxides AOs$_2$O$_3$ (A=Cs, Rb, and K) has attracted so much attention, because the geometric spin frustration inherent to their pyrochlore crystal structures is supposed to give rise to unconventional superconductivity via magnetic spin fluctuations. Until now experimental results suggest, however, that CsOs$_2$O$_6$ ($T_c = 3.3$ K) and RbOs$_2$O$_6$ ($T_c = 6.3$ K) are fully gapped s-wave superconductors. On the other hand, the experimental data of KOs$_2$O$_3$ ($T_c = 9.6$ K) show somewhat unusual behaviors, pointing out in some cases to unconventional superconductivity. In this talk we shall discuss magnetic penetration depth data of single crystals of KOs$_2$O$_3$ down to 30 mK. The data clearly indicate that KOs$_2$O$_3$ is a fully single-gapped s-wave superconductor. This implies that all of the geometrically spin-frustrated compounds known until now respond as conventional superconductors, which would suggest that spin frustration does not lead to unconventional pairing as expected.

1:51PM P8.00012 Muon spin relaxation and hyperfine-enhanced $^{141}$Pr nuclear spin dynamics in (Pr$_x$La)$_3$Os$_2$Sb$_2$ and Pr(Oh,Ru)$_3$Sb$_2$ by Dipole-Coupled Nuclear Spins. LEI SHU, D.E. MACLAUGHLIN, U. Calif., Riverside, W. HIGEMOTO, R.H. HEFFNER, K. OHISHI, T.U. ITO, JAEA, Tokai, Japan, Y. AOKI, T. YUNISHIMA, Y. YONEZAWA, S. SANADA, D. KIKUCHI, H. SATO, TMU, Tokyo, Japan, K. ISHIDA, Kyoto U., Kyoto, Japan, R. KADONO, A. KODA, KEK, Ibaraki, Japan, O.O. BERNAL, Calif. State U., Los Angeles, H. SUGAWARA, U., Tokushima, Tokushima, Japan, N.A. FREDERICK, W.M. YUHAS, T.A. YESLES, T. YANAGISAWA, M.B. MAPLE, U. Calif., San Diego — The longitudinal-field muon relaxation experiments have been carried out in the Pr$_x$La$_3$Os$_2$Sb$_2$ and Pr(Oh,Ru)$_3$Sb$_2$ alloy systems. At low temperatures, the dynamic fluctuations are involved in muon relaxation in addition to the contribution from a distributions of static muon local fields. The temperature and concentration dependencies of the muon damping rate $\Lambda$ indicate that this dynamic contribution is due to $^{141}$Pr nuclear magnetism, which is enhanced by hyperfine coupling to the Pr$^{3+}$ Van Vleck susceptibility. Further evidence comes from the field dependence of $\Lambda$, which is in reasonable agreement with the modified model for muon spin relaxation by dipole-coupled nuclear spins.

2:03PM P8.00013 Andreev Spectroscopy Study of the Heavy-Fermion Superconductor PrOs$_2$Sb$_12$. C.S. TUREL, I. FRIDMAN, J.Y.T. WEI, University of Toronto, W.M. YUHAS, M.B. MAPLE, University of California at San Diego — The discovery of superconductivity in the heavy-fermion material PrOs$_2$Sb$_12$ has attracted widespread interest. In particular, there is evidence for multiple superconducting order parameters, at least one of which is believed to have nodes. We present Andreev spectroscopy data, down to 80 mK and up to 2.5 T, taken using ballistic point contacts made with Pt-Ir tips on single crystals of PrOs$_2$Sb$_12$. Pronounced zero-bias conductance peaks (ZBCPs) seen in the differential conductance spectra, show the existence of nodes in the order parameter. The magnetic field and temperature evolution of the spectra were studied to track how the pairing symmetry evolved, allowing us to map out the order parameter phase diagram. We observed that the ZBCP’s vanished at a magnetic field $H^*$, lower than the upper critical field, $H_c2$. This implies a field-driven change in the nodality of the order parameter at $H^*$, suggesting there are multiple superconducting phases with different pairing symmetries in PrOs$_2$Sb$_12$.

Acknowledgements: This work was supported by NSERC, CFI/OIT, Canadian Institute for Advanced Research and U. S. Department of Energy under Grant No. DE-FG02-04ER46105.

Wednesday, March 7, 2007 11:15AM - 1:39PM_

Session P9 DMP: Superconductivity: Synthesis Colorado Convention Center Korbel 1D

11:15AM P9.00001 ABSTRACT WITHDRAWN

11:27AM P9.00002 Superconducting properties of the hexagonal layered molybdenum carbide $\eta$-Mo$_3$C$_2$. K. YAMAURA, Q. HUANG, M. AKAISHI, T. TAKAYAMA-MUROMACHI, National Institute for Materials Science, Japan — Superconductivity of $\eta$-Mo$_3$C$_2$ ($T_c=8.5$K) was reported in 1960s, while detailed superconducting and structure properties remained uncertain probably because those were complicated somewhat by the carbon non-stoichiometry, partially thermal decomposition, and so on. Recently, we found the degree of problems is fairly low. In the as-grown rod is not single phase. The large single crystals of La$_2$CuO$_2$ have $T_c=8.5$K, which is close to that for the comparable Pr$_x$Mo$_3$C$_2$ [1]. A significant layered character was found in the structure, which comprises edge-sharing MoO$_6$ octahedra sheets and $\sim 50$% carbon occupied blocks. Magnetic characterization revealed the Ginzburg-Landau parameter of $\lambda^*$ is $\sim 26$, which is close to that for the comparable $T_c$ compound $\lambda^*$, $\sim 21$, but less than a half of that for $\lambda^*$ for MgCu$_2$ ($\sim 54$).

12:03PM P9.00005 Refined crystal growth and characterization of the high-Tc superconductor HgBa2CuO4+δ . YUAN LI, Department of Physics, Stanford University, NEVEN BARSIC, Stanford Synchrotron Radiation Laboratory, GUILAUME CHABOT-COURTIER, Department of Applied Physics, Stanford University, YONG-CHAN CHO, Stanford Synchrotron Radiation Laboratory, GERT JAN KOSTER, G-LAM, Stanford University, GUICHUAN YU, Department of Physics, Stanford University, XUDONG ZHAO, Department of Physics, Jiilin University, MARTIN GREVEN, Department of Applied Physics, Stanford University — Among the high-Tc superconductors, HgBa2CuO4+δ (Hg1201) is one of the most desirable systems for experimental study due to its relatively simple structure and high Tc. For quantitative experimental work, it is necessary to grow sizeable, high-quality crystals, and to obtain fine oxygen/doping control. Here we report on our most recent improvements in the growth and characterization of Hg1201, leading to further improved sample quality. Our new results include charge transport, magnetic susceptibility, and x-ray photoelectron spectroscopy (XPS) measurements.

12:15PM P9.00006 Carrier density control and phase diagram of Li2ZrNCl superconductors . YASUJIRO TAGUCHI, ATSUSHI KITORA, YOSHIHIRO IWASA, Institute for Materials Research, Tohoku University — We succeeded in synthesizing a series of Li2ZrNCl samples with controlled doping level x (0 ≤ x ≤ 0.3) which are confirmed to be of single phase by means of synchrotron x-ray diffraction measurements. We found that Tc rapidly increases upon reducing Li concentration below x=0.12 to reach the maximum value of 15.2 K at x=0.06, and that a superconductor-to-insulator transition (SIT) is encountered at x=0.05 due to the Anderson localization effect. Such an increase in Tc on the verge of SIT seems to be difficult to explain by the conventional theory, but may be indicative of the charge fluctuation contribution to superconductivity in low-carrier-density systems.

12:27PM P9.00007 Strain induced morphological instability of epitaxial YBa2Cu3O7−δ films deposited on LAO and STO . PRIYA.V. CHINTA, O. LOZANO, P. WADEKAR, Q.Y. CHEN*, X.M. WANG, J.R. LIU, W.K. CHU, Dep. of Physics and TsSUH, University of Houston, TX. H.W. SEO, Dep. of Physics, University of Arkansas, AR. L.W. TAY, H.M. HUANG, Y.L. CHENG, C.P. SUN, H.D. YANG, Dep. of Physics and Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, NSYSU, Taiwan — Surface morphological instabilities in superconducting YBCO films have not yet been fully understood because of the intractably involved underlying driving forces. In this work we attempted to pin-point the lattice mismatch effect on the evolution of surface morphology for YBCO films on LaAlO3 and SrTiO3 substrates grown epitaxially by DC magnetron sputtering or laser ablation. The initial root-mean-square roughness of the samples studied was about 10-15 nm. This value was reduced to 1-3 nm after the samples were subjected to a 30-keV (Ar)+ gas cluster ion beam (GCIB) sputtering at right angle to a dose of 2×10^16 cm−2. Controlled annealing of these smoothened films in flowing O2 atmosphere was then conducted at different temperatures and time periods, upon which consistent surface roughening (SR) was observed. This SR is attributed to the elastic strain of lattice-mismatch between the film and substrate. The effects of interface coherency on such phenomenon will be discussed. *Also with NSYSU

12:39PM P9.00008 Disordered superconducting films in strong magnetic fields , YONATAN DUBI, Physics Department, Ben-Gurion University, Beer Sheva 84105, Israel, YIGAL MEIR, YSHAI AVISHAI, Physics Department and the Ilse Katz Center for Meso and Nano-scale Science and, Ben-Gurion University, Beer Sheva 84105, Israel — Experimental studies of magneto-resistance in disordered superconducting thin films reveal an abundance of unexpected results, such as a huge peak in the magneto-resistance on the insulating side of the superconductor-insulator transition which evolves as the field is tilted, and traces of superconducting correlations that survive well above the transition. Recently, a theory that accounts for these effects was suggested, in which it is postulated that (i) well-separated SC islands are formed in the disordered film, and (ii) their size and strength diminishes with magnetic field. In this work we present extensive numerical calculations which support these conjectures, by means of a locally self-consistent solution of the BdG equations in the presence of disorder and tilted magnetic field. Simple phenomenological arguments from percolation theory are then used to explain various experimental findings, such as the non-monotonic magneto-resistance in parallel field and the relation between the critical field and the magnetic field tilt angle.

12:51PM P9.00009 Investigation of tunneling density of state of FSF trilayers . JUN HYUNG KWON, JEWOOK PARK, SEONG KOOK CHOI, KOOKRIN CHAR, Center for Strongly Correlated Materials Research, Dept. of Physics and Astronomy, P.G. SANGIOR-, M.R. BEASLEY, Dept. of Applied Physics, Stanford University — Unconventional superconductivity such as π-state and long range triplet superconductivity may arise in an FSF trilayer structure, depending on the relative directions of the magnetization of two ferromagnetic layers. In order to observe such unconventional states by measuring tunneling density of state(DOS) of FSF structure, we fabricated Al(12nm)/AlOx/CoFe(2.5nm)/Nb(20,30,40nm)/NiFe(10nm) using stencil mask method in a cross-strip geometry. In order to easily change magnetization direction of the magnetically soft NiFe layer, we further etched the last NiFe layer into a square shape by ion beam milling. We will present magnetic force microscope(MFM) image of the NiFe layer as its magnetization tilt angle.

1:03PM P9.00010 Magnetic Field Enhanced Insulating Behavior in Thin Films with Local Cooper Pairing , K. H. SARWA B. TAN, KEVIN A. PARENDO, University of Minnesota, Z. OVADYAHU, The Hebrew University, A. M. GOLDMAN, University of Minnesota — The effects of a perpendicular magnetic field on insulating amorphous indium oxide thin films exhibiting local superconductivity may arise in an FSF trilayer structure, depending on the relative directions of the magnetization of two ferromagnetic layers. In order to observe such unconventional states by measuring tunneling density of state(DOS) of FSF structure, we fabricated Al(12nm)/AlOx/CoFe(2.5nm)/Nb(20,30,40nm)/NiFe(10nm) using stencil mask method in a cross-strip geometry. In order to easily change magnetization direction of the magnetically soft NiFe layer, we further etched the last NiFe layer into a square shape by ion beam milling. We will present magnetic force microscope(MFM) image of the NiFe layer as its magnetization tilt angle.

1:15PM P9.00011 Electrical transport properties of ultrathin superconducting Pb films . R.P. PANGULURI, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201, M.M. OZER, Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996, J.R. THOMPSON, H.H. WEITERING, Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996;Condensed Matter Sciences Division, ORNL, Oak Ridge, TN 37831, B.E. NADGORNAY, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201 — We present electrical transport properties of metallic ultra thin epitaxially grown Pb (111) films on Si (111) substrate. We observed a reduced superconducting transition temperature from bulk Pb using electrical resistivity measurements and deduced the temperature dependence of out-of-plane critical magnetic fields from the sheet resistance R as a function of the applied magnetic field. These results are consistent with M. M. Ozer et al., obtained by magnetic techniques. We identified the mean field temperature and current densities from I-V curves in zero magnetic field. We explored the possible presence of Kosterlitz-Thouless transition (Tc,KT) in this system. We discuss these results based on the Ginzburg-Landau Coloumb-Gas (GLCG) model for 2D vortex fluctuations. 1. M. M. Ozer, J. R. Thompson, and H. H. Weitering, Nature Physics, 2, 173 (2006).
1:27PM P9.000012 The effect of magnetic field on superconductivity in ultrathin amorphous Pb films with paramagnetic impurities, ASHWANI KUMAR, H. JEFFREY GARDNER, PENG XIONG, Department of Physics and MARTECH, Florida State University — We report on a systematic study of the effect of applied magnetic fields on superconductivity in ultrathin amorphous Pb films containing various amounts of paramagnetic impurities. The Pb film, along with a 1 nm thick Sb buffer layer, was quench-condensed onto a Si substrate with pre-deposited Au contacts in a modified dilution refrigerator. Cr impurities were then deposited onto the Pb film by heating a NiCr wire at a fixed current. Both the Pb thickness (thus its Tc) and the Cr density can be varied, and electrical measurements can be performed at each field in perpendicular magnetic fields up to 8 T, all in situ. The reduction of the Pb Tc with increasing Cr density is well described by the Abrikosov-Gorkov theory. The application of perpendicular magnetic fields did not result in any suppression of the pair-breaking effect by the Cr impurities, i.e., field enhanced superconductivity, on several samples covering a wide range of Pb thicknesses and Cr densities. The pronounced reentrant behavior found in the magnetic field-tuned transitions in pure Pb films1 was progressively suppressed by increasing Cr impurities. 1 J.S. Paker et al., Europhys. Lett. 75, 950 (2006).

Wednesday, March 7, 2007 11:15AM - 2:15PM – Session P12 GMAG DMP FIAP: Focus Session: Spin-Orbit Coupling Colorado Convention Center Korbel

11:15AM P12.00001 Electrical manipulation of spin-orbit coupling in semiconductor heterostructures1, VANESSA SIH, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Spin-orbit coupling provides a pathway for electrically initializing and manipulating electron spins. This coupling creates momentum-dependent spin-splittings related to the inversion asymmetries of the semiconductor heterostructure. We demonstrate that we can regulate these spin-splittings in semiconductor epilayers with strain[2] and in heterostructures using quantum confinement and orbital quantization[3]. These spin-splittings provide a mechanism for electrically generating, studied in isolation without magnetic materials or magnetic fields. Using strain, rotation microscopically current-induced spin polarization and the spin Hall effect have been observed in bulk semiconductors and in a two-dimensional electron gas confined in (110) AlGaAs quantum wells[4]. In contrast to measurements on bulk systems, the data for the quantum wells reveal that the spin Hall profile exhibits a complex structure and that the current-induced spin polarization is out-of-plane. The current-induced spin polarization is dependent on the direction along which the electric field is applied, reflecting the anisotropy of the spin-orbit interaction. More recently, we demonstrate that the observed spin accumulation due to the spin Hall effect is due to a bulk electron spin current[5]. Channels with transverse arms allow us to observe that this spin current can drive spin transport over macroscopic distances in bulk GaAs.

1 This work was supported by ARO, DARPA/DMEA, NSF and ONR.

11:51AM P12.00002 Spin generation by strong inhomogeneous electric fields, ILYA FINKLER, HANS-ANDREAS ENGEL, EMMANUEL RASHBA, BERTRAND HALPERIN, Harvard University — Motivated by recent experiments [1], we propose a model with extrinsic spin-orbit interaction, where an inhomogeneous electric field \( E \) in the \( x \)-\( y \) plane can give rise, through nonlinear effects, to a spin polarization with non-zero \( s_z \), away from the sample boundaries. The field \( E \) induces a spin current \( j_y = \hat{z} \times (\alpha j_x + \beta E) \), where \( j_x = E \) is the charge current, and the two terms represent, respectively, the skew scattering and side-jump contributions. [2]. The coefficients \( \alpha \) and \( \beta \) are assumed to be \( E \)- independent, but conductivity \( \sigma \) is field dependent. We find the spin density \( s_z \) by solving the equation for spin diffusion and relaxation with a source term \( \nabla \times j_y \). For sufficiently low fields, \( j_y \) is linear in \( E \), and the source term vanishes, implying that \( s_z \) is zero away from the edges. However, for large fields, \( s_z \) varies with \( E \). Solving the diffusion equation in a T-shaped geometry, where the electric current propagates along the main channel, we find spin accumulation near the entrance of the side channel, similar to experimental findings [1]. Also, we present a toy model where spin accumulation away from the boundary results from a nonlinear and anisotropic conductivity. [1] V. Sih, et al, Phys. Rev. Lett. 97, 096605 (2006).

12:03PM P12.00003 Tuning of the spin-orbit interaction and resistance in two-dimensional GaAs holes via strain, BABUR HABIB, JAVAD SHABANI, ETIENNE P. DE POORTERE, MANSOUR SHAYEGAN, Department of Electrical Engineering, Princeton University, ROLAND WINKLER, Department of Physics, Northern Illinois University — We report direct measurements, via the Fourier analysis of the Shubnikov-de Hass oscillations, of the spin-orbit interaction induced spin-splitting in modulation-doped GaAs two-dimensional hole systems as a function of strain applied in the sample plane. The data reveal a remarkably strong dependence of the spin-splitting on strain, with up to about 20% enhancement of the splitting upon the application of only about 2x10^-4 strain. The results are in very good agreement with our numerical calculations of the strain-induced spin-splitting. We also show a remarkable dependence of the anisotropy of the heavy hole band on strain. Its manifestation as a change of resistance with strain implies the use of GaAs 2D holes as a sensitive piezo-resistance sensor at low temperatures.

12:15PM P12.00004 Electron transport in semiconductor heterostructures with strong spin orbit coupling, ANDREI GARCIA, DENNIS LO, DAVID GOLDHABER-GORDON, Stanford University, JASON STEPHENS, SHAWN MACK, DAVID AWSCHALOM, UC Santa Barbara — GaAs/AlGaAs two dimensional electron gases (2DEGs) have been studied extensively in the context of mesoscopic transport through devices such as quantum point contacts and quantum dots. 2DEGs in heterostructures based on InGaAs or InAs instead of GaAs provide testbeds to study similar phenomena in systems with much larger intrinsic spin-orbit coupling. Stronger spin orbit coupling provides greater ease of control of the electron spin degree of freedom, leading to applications in spintronics as well as the possibility of observing novel quantum Hall states. We present some preliminary electronic transport data on gated InGaAs 2DEGs and discuss directions for possible further experiments on nanostructures in this material.

12:27PM P12.00005 Physical factors affecting Rashba Spin-orbit coupling, CHIH-PIOA CHU, Univ. of Texas at Austin, MING-CHE CHANG, National Taiwan Normal University, QIAN NIU, Univ. of Texas at Austin — The Rashba Spin-orbital coupling plays a crucial role in charge and spin transport in semiconductor heterostructure. We study several physical parameters which may contribute to Rashba Spin-orbital coupling, including asymmetric potential barriers, quantum well inclination, effective mass, and band mixing. This may provide some insights in designing spintronic microdevices.
12:39PM  P12.00006 Spin transport and the giant Zeeman effect in systems with spin-orbit interaction. ANH NGO, SERGIO ULLG, Ohio University — Spin-orbit coupling in semiconductors provides a pathway for electrically initializing and manipulating electron spins for applications in spintronics and spin-based quantum information processing. This coupling can be regulated with quantum confinement, band structure engineering and applied fields. Here we investigate the spin-dependent transport properties of electrons in diluted magnetic two-dimensional electron gas (2DEG) systems using a scattering matrix approach. We include the Rashba spin-orbit interaction and the role of realistic magnetic barriers produced by the deposition of ferromagnetic stripes on heterostructures. We show that the quantum conductance in these systems depends on spin orientation of the incident carriers, the magnitude of spin-orbit coupling, and the giant Zeeman effect present in diluted magnetic semiconductors. We describe how all effects can be employed in the efficient control of spin polarization via the application of moderate fields.


1Supported by NSF-NIRT

12:51PM P12.00007 Spin-Orbit Coupling in AlGaN/AlN/GaN Heterostructures with a Polarization Induced Two-Dimensional Electron Gas. H. CHENG, C. KURDAK, Physics Dept, Univ of Michigan, N. BIVIJKI, U. OZGUR, H. MORKOC, Dept of Electrical Engineering, Virginia Commonwealth University, V. I. LITVINOV, V. I. M. NIPS, SIEMENS Corporation, Irvine, CA 92618 — Spin-orbit coupling is investigated by weak antilocalization and Shubnikov-de Haas measurements in wurzite AlGaN−xN/GaN heterostructures with a polarization induced two-dimensional electron gas. By employing the persistent photoconductivity effect and by using five different heterostructures with different AI compositions, we cover a carrier density range extending from 0.8 × 10^{12} cm^{-2} to 10.6 × 10^{12} cm^{-2}. We determine electron splitting energies for different carrier densities by analyzing the weak antilocalization measurements using the Iordanskii, Lyanda-Geller, and Pikus theory. We find the spin splitting energies do not scale linearly with the Fermi wavevector k_{F} at high carrier densities. By fitting the spin splitting energies to a form$$E_{SO}(\gamma, k_{F}^{2}) = 2\hbar\omega_{s}(\gamma, k_{F}^{2}) + \hbar\gamma_{SO}$$, we extract linear and cubic spin-orbit coupling strengths$$\gamma_{SO} = 5.13 \times 10^{-13}$$ eV m and$$\gamma_{SO} = 1.2 \times 10^{-13}$$ eV m, respectively. The cubic spin-orbit coupling parameter is purely due to the bulk inversion symmetry of the wurzite crystal and has not been previously measured for the GaN system.

1:03PM P12.00008 A Study of Dresselhaus and Rashba Effects in InSb/InAlSb Heterostructures via Anti-Weak Localization Measurements. ARUNA DEDIGAMA, DILHANI JAYATHILAKA, SHEENA MURPHY, MADHAVIE EDIRISOOYI, NITI GOEL, TETSUYA MISHIMA, MICHAEL SANTOS, University of Oklahoma, C-SPIN COLLABORATION — The InSb/InAlSb system has both the largest Dresselhaus effect (due to bulk inversion asymmetry) and Rashba effect (due to structural inversion asymmetry) of the III-V semiconductor family. Both mechanisms contribute to electronic spin splitting, even in zero applied field. While the Dresselhaus effect is purely materials specific, the Rashba interaction is less well understood with both the electric field at the interface and the discontinuity due to the barrier predicted to play significant roles. Standard measurements of the zero field spin splitting however, are usually performed at high field where Zeeman effects and higher subband occupancy become problematic. In this talk we will present our results in extremely low fields using anti-weak localization (AWL) measurements where these complications are absent. We report on systematic measurements of the Dresselhaus and Rashba interactions on a series of InSb/InAlSb heterostructures, where carrier density, dopant density and the Al concentration in the barrier have all been varied to extract the role of each in the strength of the spin-orbit coupling.

1:15PM P12.00009 Spin interference effect in a triangular loop array fabricated in (001)In_{0.53}Ga_{0.47}As/In_{0.33}Al_{0.67}As quantum wells. HIROSHI OKUTANI, GSIST, Hokkaido University, TAKA AKI KOGA, GSIST, Hokkaido University & CREST, JST, YOSHIKAI SEKINE, NTT BRL, NTT Corporation — We report, for the first time, the spin interference (SI) effect in a triangular loop arrays fabricated in (001)In_{0.53}Ga_{0.47}As/In_{0.33}Al_{0.67}As quantum wells (QW). Previously [1], we studied the SI effect in a square loop array, where the sides of the squares are either parallel or perpendicular to the c axis and the effective magnetic field due to all spin-orbit effects, $$B_{TOT}$$, is given either by the sum ($$B_{R} + B_{P}$$) or by the difference ($$B_{R} - B_{P}$$) between the Rashba and Dresselhaus fields, which makes the analysis relatively simple. Though the situation is more complex for a triangular loop array, including both the Rashba and Dresselhaus terms predicts clear difference in the SI patterns between the two following situations: the bases of the triangles in the array are placed parallel/perpendicular to the c axis. This finding is being confirmed experimentally. [1] T. Koga et al., Phys. Rev. B 70, 161302(R) (2004); ibid. 74, 041302(R) (2006).

1:27PM P12.00010 Spin and charge optical conductivities in spin-orbit coupled systems. JESUS A. MAYOTRENA, CCMC-UNAM, Ensenada B.C., Mexico, CATALINA LOPEZ-BASTIDAS, CCMC-UNAM, FRANCISCO MIRELES, CCMC-UNAM, Ensenada, B.C., Mexico — Spin-orbit interaction (SOI) in systems lacking inversion symmetry is a phenomenon with great potential in the development of spintronic-based devices. Since the celebrated proposal by Datta and Das, of a spin-FET relying on the tunability of the Rashba SOI strength through electrical gating, there has been a remarkable attention in the search for new ways of manipulating electron spins without employing ferromagnetic materials and/or external magnetic fields. In this work we study the frequency dependent spin- and charge- conductivity tensors of a two-dimensional electron gas (2DEG) with both Rashba and Dresselhaus spin-orbit interaction. We show that the spectral behavior of the spin and charge response due to the angular anisotropy of the spin-splitting energy is strongly influenced by the strength of the spin-orbit interaction. The new spectral structures open the possibility for control of the spin and charge optical conductivities.

1:39PM P12.00011 Spin interference effects in a 2D-hole ring with spin-orbit interaction. ALEXEY KOVALEV, MARIO BORUNDA, JAIRIO SINOVA, Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA — We study the quantum interference effects in one-dimensional heavy hole (HH) rings in spin-orbit coupled hole (QH) quantum wells. The influence of the spin-orbit interaction strength on the transport is investigated analytically and numerically. The analytical results allow us to explain the interference effects as a signature of Berry phases. We compare our results with the previous studies on the electron Rashba systems and find more rapid oscillations as a function of the spin-orbit strength. The structures with stronger signature of the spin-orbit strength can lead to more sensitive spintronic devices that enable observation of quantum interference effects and control of spin at mesoscopic scales.

1:51PM P12.00012 Exchange energy and generalized polarization in the presence of spin-orbit coupling in two dimensions. STEFANO CHESI, GABRIELE F. GIULIANI, Department of Physics, Purdue University — We discuss the concomitant effects of the exchange energy and the spin-orbit interaction in a homogeneous system of interacting electrons in two spatial dimensions. This work extends the mean-field method originally developed in the case of Rashba spin-orbit to a more general form of spin-orbit interaction. The mean-field phase diagram and spin response for a number of representative cases are discussed. Our theory is rigorous in the high-density limit of the paramagnetic phase, where it can be expressed in terms of a generalized fractional electronic polarization. We show that in many cases, the effect of the exchange is to quench, rather than enhance, the generalized polarization induced by the spin-orbit coupling. Our results account qualitatively for the findings of recent experimental investigations.
2:03PM P12.00013 High density limit of the correlation energy of a two dimensional electron liquid in the presence of Rashba spin-orbit. GABRIELE F. GIULIANI, STEFANO CHESI, Department of Physics, Purdue University — We obtain analytic expressions for the high density limit of the correlation energy of a two dimensional electron liquid in the presence of Rashba spin-orbit. As a byproduct we have derived an analytic expression for the dependence of the ring diagrams contribution to this quantity on the fractional spin polarization of the system in the absence of spin-orbit. We will show that the latter is not properly represented by current standard interpolation formulas obtained from Monte-Carlo calculations.

Wednesday, March 7, 2007 11:15AM - 2:03PM –
Session P13 DMP GMAG: Focus Session: High-Tc Cuprates and Nickelates Colorado Convention Center Korbel 4C

11:15AM P13.00001 Enhanced polaron formation, suppression of superconducting $T_c$, and the isotope effect in the Hubbard model with phonons1, ALEXANDRU MACRIDIN, University of Cincinnati — Using a dynamical cluster quantum Monte Carlo approximation we investigate the effect of dynamical Holstein, buckling and breathing phonons on the physics of the 2D Hubbard model at small doping. For all three phonon modes the interplay of electronic correlations and the electron-phonon interaction produces two competing effects, an enhancement of the effective $\delta$-wave pairing interaction and a strong suppression of the single-particle quasiparticle weight. Due to the later effect we find that Holstein, buckling and breathing phonons suppress superconductivity in the region of parameter space relevant for cuprate superconductors. The renormalization of the single- particle propagator, associated with polaron formation, is significantly enhanced by the presence of antiferromagnetic correlations. Moreover, as a complementray effect, the electron-phonon scattering strongly enhances the spin correlations at finite doping, showing a synergistic interplay between the electron-phonon coupling and antiferromagnetic correlations. The suppression of superconductivity due to polaron formation can explain the isotope effect observed in cuprates. We find a positive and large isotope exponent in the underdoped region where the antiferromagnetic correlations are strong and a small positive isotope exponent in the optimally doped region, in agreement with experiment.

Supported by: CMSN DOE DE-FG02-04ER46129 and NSF DMR-0312680

11:51AM P13.00002 The effect of strong impurity scattering on superconductivity in the 2D Hubbard model1, ALEXANDER KEMPER, University of Florida, THOMAS MAIER, Oak Ridge National Laboratory, MARK JARRELL, University of Cincinnati, CHENG HAI-PING, University of Florida — We study the effect of strong impurity scattering in the two-dimensional Hubbard model to model the effect of Zn substitution in the cuprates, using the dynamical cluster quantum Monte Carlo framework. The superconducting $T_c$ is strongly suppressed by impurity doping, while the spin susceptibility indicates moment formation. We will discuss the dependence of $T_c$ on the strength of the impurity scattering potential, and by investigating the properties of sites neighboring the impurity, the relevance to the experimental STM image of Zn impurity in cuprates.

1DOE grant DE-FG02-02ER45995, NSF DMR-0312680, and the Center for Nanophase Materials Sciences which is sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. Department of Energy

12:03PM P13.00003 Exact thermodynamics of pairing and charge-spin separation in Hubbard nanoclusters. TUN WANG, Department of Physics, University of Connecticut, ARMEN KOCHARIAN, Department of Physics and Astronomy, California State University, GAYANAH FERNANDO, KALUM PALANDAGE, Department of Physics, University of Connecticut, JIM Davenport, Computational Science Center, Brookhaven National Laboratory — An exact thermal studies of charge-spin separation, pairing fluctuations and pseudogaps are carried out by exact diagonalization of 4-site, frustrated (three dimensional) tetrahedral Hubbard and planar (2x4) clusters. Our exact results for 4-site cluster strongly suggest the existence of a quantum critical points in small Hubbard clusters for particle-particle/hole pair binding, antiferromagnetism, unsaturated and saturated ferromagnetism. Exact studies of larger planar and three dimensional Hubbard clusters yield more intriguing insight supporting the analytical results obtained for the 4-site clusters. Our microscopic theory reproduces electron pairing correlations, phase separation and magnetism in clusters, small nanoparticles, and, surprisingly, in transition metal oxides and high $T_c$ doped cuprates. Theory describes also the effect of pressure on the superconducting transition temperature, the presence of a dormant magnetic state in a narrow region of doping and variation of spin pseudogap with doping level, etc.

12:15PM P13.00004 Field Induced Suppression of the Resonance Mode in N-type High-$T_c$ Cuprate Pr$_{0.8}$La$_{0.2}$CuO$_4$ ($T_c = 24K$)1, STEPHEN WILSON, University of Tennessee — We discuss the results of our recent inelastic neutron scattering experiments probing the magnetic field dependence of the resonance mode in an electron-doped high-$T_c$ cuprate. The resonance mode in the high-$T_c$ superconductors is a magnetic excitation widely believed to be fundamentally connected to the superconducting mechanism. The mode itself appears only below $T_c$ in optimally-doped cuprates, and its characteristic energy follows the universal relation $E_{Resonance} \sim 5.8k_B T_c$ in all classes of cuprate systems. Using a c-axis aligned magnetic field, superconductivity in the electron-doped cuprate, Pr$_{0.8}$La$_{0.2}$CuO$_4$ (PLCCO), can be completely suppressed with an experimentally realizable field of ~9 T at 2 K. This fact combined with the recent discovery of the resonance mode in this PLCCO system, allows, for the first time, an experimental observation of the evolution of the resonance mode as a cuprate system is driven into its field-suppressed ground state. We will present such a study in a nearly optimally-doped sample of PLCCO ($T_c = 24K$). The simultaneous emergence under field of static antiferromagnetic (AF) order at the commensurate AF ordering wavevector will also be discussed along with the influence of a c-axis field on low energy excitations in this system. Changes in magnetism coupled to the suppression of the superconducting phase in this PLCCO system will be given particular focus.

This research is supported by NSF DMR-0453804.

12:51PM P13.00005 Local Electronic Structure of Bi2Sr2CaCu2O8 near Oxygen Dopants: A Window on the High-Tc Pairing Mechanism1, YAO HE, PETER HIRSCHFELD, HAI-PING CHENG, University of Florida — The cuprate material Bi$_2$Sr$_2$CaCu$_2$O$_8$ (BSCCO-2212) is believed to be doped by a combination of cation switching and excess oxygen. The interstitial oxygen dopants are of particular interest because scanning tunneling microscopy (STM) experiments have shown that they are positively correlated with the local value of the superconducting gap, and calculations suggest that the fundamental attraction between electrons is modulated locally. In this work, we use density functional theory to try to ascertain which locations in the crystal are energetically most favorable for the O dopant atoms, and how the surrounding cage of atoms deforms. Our results provide support for the identification of STM resonances at -1.0 eV with dopant interstitial O atoms, and show how the local electronic structure is modified nearby.

Supported by DOE under DE-FG02-97ER45660DE-FG02-02ER45995, NSF/DMR/ITR/DMR-032553, ONR/N00014-04-0060, and DOE/DEFG02-05ER46236

1Supported by DOE under DE-FG02-97ER45660DE-FG02-02ER45995, NSF/DMR/ITR/DMR-032553, ONR/N00014-04-0060, and DOE/DEFG02-05ER46236
1:03PM P13.00006 Metal to insulator transition and ground state electronic structure of La$_2$-$x$Sr$_x$CuO$_4$.

T.C. SCHULTHESS, Oak Ridge National Laboratory, W.M. TEMMERMAN, Z. SZOTEK, Daresbury Lab., P.R.C. KENT, U. of Tennessee — We use the self-interaction corrected local spin-density (SIC-LSD) method to study the ground state electronic structure of La$_2$-$x$Sr$_x$CuO$_4$ as a function of Sr doping $x$. SIC-LSD is a parameter free method based on Density Functional Theory that has proven reliable for the study of strongly correlated electron systems. It is introduced via the virtual crystal approximation by linearly mixing the La and Sr potentials. In our calculations, we find that the nature of Cu-2$d_{2-2y}$ orbital changes character with varying Sr concentration. In the under-doped regime, one of the Cu-2$d_{2-2y}$ orbitals per atom is fully occupied and localized on the Cu site, leading to the formation of magnetic moments on Cu aligned antiferromagnetically in the CuO$_2$ plane. Sr doping introduces holes mainly into the O-p bands and the system is a doped charge transfer insulator. In the over-doped regime, the Cu-2$d_{2-2y}$ orbitals are band-like and not spin-split. The moments on the Cu atoms vanish and the system is a nonmagnetic metal. In the orthorhombic structure, the transition from localized to band-like Cu-2$d_{2-2y}$ states occurs at about 18% Sr doping, i.e. within the region of optimal doping for superconductivity. We find a similar behavior if the calculations are performed with the idealized tetragonal structure.

1:15PM P13.00007 A pressure induced inducer-to-metal critical point in the copper-oxides.

TANJA CUK, Stanford University, VIKTOR STRUZHCHIN, Carnegie Institution of Washington, THOMAS DEVEREAUX, University of Waterloo, ALEXANDER GONCHAROV, Carnegie Institution of Washington, CHRISTOPHER KENDZIORA, Naval Reseach Laboratory, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, HOKWANG MAO, Carnegie Institution of Washington, ZHI-XUN SHEN, Stanford University — The presence of a quantum critical point inside the superconducting dome is a novel ideal unifying high-Tc superconductivity in the copper-oxides with that of other unconventional superconductors in strongly correlated materials. Experimental progress, however, has been difficult since superconductivity protects it from most direct measurements. Yet, the tuning parameter of all efforts to date has been chemical doping, which varies crystal fields, electron-phonon, and electron-electron interactions with potentially very different physical metrics. We report pressure tuned Raman and x-ray scattering data revealing an inducer-to-metal critical point near 20GPa with anomalies in six physical quantities: electronic Raman background, phonon lineshape and temperature dependence, density dependent behavior of phonon and magnon frequencies, and a subtle structural change in the c-axis. We also suggest why this critical point may be near optimal doping in the high-Tc phase diagram.

1:27PM P13.00008 ABSTRACT WITHDRAWN

1:39PM P13.00009 Suppression of charge stripes in highly strained, epitaxial La$_{5/3}$Sr$_{1/3}$NiO$_4$ films.

CHANGKUN XIE, BARRETT WELLS, Department of Physics, University of Connecticut, CT 06269-3046, FEIZHOU HE, Canadian Light Source, University of Saskatchewan, Saskatoon, Canada, ARNOLD MOODENBAUGH, Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973 — We have successfully grown epitaxial La$_{5/3}$Sr$_{1/3}$NiO$_4$ films with a small crystalline mosaic using pulsed laser deposition. Using synchrotron radiation, the x-ray diffraction peaks associated with charge stripes have been successfully observed for relatively thick films with little strain. Anomalies due to the charge-ordering transition have been examined using four-point probe resistivity measurement. We also have produced highly strained films with the same total thickness through the use of multilayers of La$_{5/3}$Sr$_{1/3}$NiO$_4$ alternating with SrTiO$_3$. These films remain under in-plane tension. A thorough search for the stripe charge peaks in the strained multilayers has been negative; the stripes appear to be suppressed under these conditions. This suggests that electron-lattice interactions are critical for the formation of stripe phases. This work is supported through NSF DMR-0239667. Some data was taken at the National Synchrotron Light Source, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Division of Materials Sciences and Division of Chemical Sciences.

1:51PM P13.0010 Study of the antiferromagnetism in electron-doped cuprate superconductors with disorder.

C.S. TING, XIN-ZHONG YAN, QINGSHAN YUAN, Texas Center for Superconductivity, University of Houston — On the basis of the Hubbard model, we study the antiferromagnetic (AF) properties in electron-doped cuprates using the fluctuation-exchange approach. Taking into account the spin fluctuations in combination with the impurity scattering effect due to the randomly distributed dopant-atoms, we formulate the theory of antiferromagnetism in the system. By self-consistently solving the integral-equations for the Green’s function, the Neel’s temperature is determined by the condition that the Goldstone mode from the transverse spin susceptibility first appears as the temperature is lowered. Our numerical calculation shows that the Goldstone mode always is pinned at $\pi$‘s, insensitive to the doping level. We also calculate the onset temperature of the pseudogap formation which is due to the antiferromagnetic fluctuations, the single particle spectral density, the Fermi surface evolution with doping concentration, and the staggered magnetization. It is shown that the results obtained by the present approach are in very good agreement with the experiments. In the present approach, the density of states (DOS) of the antiferromagnetic phase exhibits a zero-energy peak in the under-doped region.

Wednesday, March 7, 2007 11:15AM - 2:15PM –
Session P14 MAG DMP: Focus Session: Magnetic Nanostructures I Colorado Convention Center Korbel 4D

11:15AM P14.00001 Coercivity of nanometer size Ni granular films as a function of temperature, grain size and dipolar interaction.

R. DAS, A.F. HEBARD, University of Florida, A. GUPTA, D. KUMAR, North Carolina A&T State University — The influence of temperature, grain size and dipolar interaction (DI) on coercive field $H_c$ determined from hysteretic magnetization loops has been studied in nanometer size Ni granular films embedded in an insulating AIO$_x$ host matrix. Single layer (SL) and multilayer (ML) samples were grown using pulsed laser deposition by sequential deposition from AIO$_x$ and Ni targets. The Ni film thickness $d$, and hence the average grain size, is varied over the range of 3nm to 60nm. In the ML samples, the Ni layers are separated by 3nm-thick AIO$_x$. At low temperatures $H_c(d)$ exhibits a peak at a crossover thickness $d_c$ delineating single domain (SD) from multi domain (MD) behavior. The ML sample has a smaller $d_c$ because of the increase in magneto static energy due to an increased DI associated with a greater number of nearest neighbors. In the SD region common to both samples, the $H_c$‘s are considerably higher for ML samples compared to those for SL samples. This effect can be understood in terms of collective dynamics of the interacting particles [1]. Surprisingly, $H_c(T)$ shows the well known Stoner-Wohlfarth square root temperature dependence in the MD region for both SL and ML samples. Even more surprising is the unexpected oscillatory dependence of $H_c(d)$ in the MD region for the SL samples. [1] C. Djurberg et al., Phys. Rev. Lett. 79, 5154 (1997).
The sample under investigation. We will discuss their manifestations in both simulations and experimental data. High magnetic field gradient of the MRFM probe micromagnet. The presence of the high field gradient imposes unusual conditions on the FMR resonance in MRFM. MRFM is a novel scanned probe technique based on mechanical detection of magnetic resonance. Its extreme sensitivity originates partially from the excitations in thin ferromagnetic samples in the presence of a nonuniform magnetic field to our FMR data obtained with Magnetic Resonance Force Microscopy.

1:03PM P14.00002 Dynamic Hysteresis of Fe10Co90 Nanoparticle Compacts, K. M. Chowdary, Dept. of Physics and Astronomy, Bucknell University, Lewisburg PA 17837, S. A. Majetic, Dept. of Physics, Carnegie Mellon University, Pittsburgh PA 15213 — The time-dependent magnetic response of composites made of consolidated Fe10Co90 nanoparticles was measured and modeled. 200 nm particles with average grain size 20 nm synthesized by the polyol method were consolidated to 95% theoretical density by plasma pressure compaction. Power loss, complex permeability, and coercivity were extracted from dynamic minor hysteresis loops measured over a range of temperatures (77 K – 873 K) and frequencies (100 Hz – 100 kHz) for toroidal samples. When the data were scaled relative to the peak frequency of the imaginary permeability, universal behavior was observed, with two distinct components. This behavior is explained through simulations of the Néel-Brown thermal aftereffect in which a time-dependent energy barrier in an Arrhenius-Néel law gives a rate equation for magnetization reversal. Quantitative attempts to match model and experiment indicate a distribution of energy barriers along with coupled and uncoupled regions in the compacted sample. The uncoupled regions limit the useful frequency range of the sample.

11:27AM P14.00002 Dynamic Hysteresis of Fe10Co90 Nanoparticle Compacts, K. M. Chowdary, Dept. of Physics and Astronomy, Bucknell University, Lewisburg PA 17837, S. A. MAJETICH, Dept. of Physics, Carnegie Mellon University, Pittsburgh PA 15213 — The time-dependent magnetic response of composites made of consolidated Fe10Co90 nanoparticles was measured and modeled. 200 nm particles with average grain size 20 nm synthesized by the polyol method were consolidated to 95% theoretical density by plasma pressure compaction. Power loss, complex permeability, and coercivity were extracted from dynamic minor hysteresis loops measured over a range of temperatures (77 K – 873 K) and frequencies (100 Hz – 100 kHz) for toroidal samples. When the data were scaled relative to the peak frequency of the imaginary permeability, universal behavior was observed, with two distinct components. This behavior is explained through simulations of the Néel-Brown thermal aftereffect in which a time-dependent energy barrier in an Arrhenius-Néel law gives a rate equation for magnetization reversal. Quantitative attempts to match model and experiment indicate a distribution of energy barriers along with coupled and uncoupled regions in the compacted sample. The uncoupled regions limit the useful frequency range of the sample.

11:39AM P14.00003 Cluster Beam Synthesis of Magnetic Nanoparticles, R. H. KODAMA, J. J. KAVICH, M. VEDPATHAK1, M. C. PETERSON, Univ. of Illinois at Chicago — Highly mono-dispersed Ni and Fe nanoparticles are produced using a cluster beam source. The source chamber is isolated from a deposition chamber using a small orifice. By balancing process gas flow, orifice size, and pumping speed we can create a high-pressure sputtering environment, suitable for nanoparticle condensation. The average beam flux and a spatial beam profile are acquired using a quartz crystal monitor with line-of-sight control. We find that the time stability of the nanoparticle flux is very sensitive to sputtering power and temperature gradients in the cluster source. AFM and TEM measurements have shown a correlation of particle size with position in the beam. Both size distribution and time stability seem to be sensitive to small perturbations in the gas flow near the sputtering source. High-Resolution TEM images indicate that the particles are randomly oriented and nano-crystalline in nature. The magnetic properties of Ni nanoparticles are measured using a SQUID magnetometer.

11:51AM P14.00004 Detection of exchange interaction in diatomic molecules by Fano resonance, JONAS FRANSSON, ALEXANDER BALATSKY, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545 — We propose a mechanism to use STM for direct measurements of the two-electron singlet-triplet exchange splitting J in diatomic molecular systems, based on the coupling between the molecule and the substrate electrons. The different pathways for electrons lead to interference effects and generate kinks in the differential conductance at the energies for the singlet and triplet. These features are related to Fano resonance due to the branched electron wave functions. Since the ratio between the tunnelling through the two atoms can be modulated by spatial movements of the tip along the surface this suggests a technique for detection of the singlet-triplet exchange splitting with STM.

12:03PM P14.00005 Measurement of Magnetic Anisotropy for Individual Atomic Spins on Surfaces, CYRUS F. HIRJIBEHEDIN, IBM Almaden Research Center, ALEXANDER F. OTTE, IBM Almaden Research Center and Leiden University, MARKUS TERNES, IBM Almaden Research Center and EPF Lausanne, CHRISTOPHER P. LUTZ, ANDREAS J. HEINRICH, IBM Almaden Research Center — We measure the effects of magnetic anisotropy on individual magnetic atoms on a thin-insulating surface. Using the inelastic electron tunneling spectroscopy capabilities of a scanning tunneling microscope, we probe the spin excitation spectra of Mn and Fe atoms adsorbed on a single copper nitride layer. Magnetic anisotropy is directly manifested as finite-energy spin excitations that exist even in the absence of a magnetic field. The effects of anisotropy are found to be relatively weak for Mn atoms but are substantially larger for Fe atoms, in which spin-orbit coupling is prominent. When a magnetic field is applied to the Fe atoms, the spin excitations shift in a manner that is strongly dependent on the direction of the applied field. These shifts in energy can be understood both qualitatively and quantitatively with a Hamiltonian containing in-plane and out-of-plane magnetic anisotropies.

12:15PM P14.00006 Ferromagnetic multipods fabricated by solution phase synthesis and hydrogen reduction, YUChENG SUI, YAO ZHAO, JUN ZHANG, SITARAM JASWAL, XINGZHONG LI, DAVID SELLMYER, Department of Physics and Astronomy and NCMN, University of Nebraska, Lincoln, NE, 68588-9113 — New functional materials might emerge if nanocrystals of higher complexity than those with simple geometries (spheres, rod, discs) could be produced. Branched nanostructures (called multipods) have attracted much attention owing to their potential as building blocks in the fabrication of complex, multi-terminal devices through self assembly. In this work, we demonstrate that ferromagnetic Co multi-branched nanostructures can be produced through the combination of solution-phase synthesis and hydrogen reduction. The CoO multipods were produced through the pyrolysis of cobalt-oleate in octadecane at 280°C in the presence of oleic acid under the protection of pure nitrogen. Arm lengths and diameters of the CoO multipods are about 30 and 10 nm respectively, and the angles between the nearest arms are 90 degrees. The multipods were assembled onto Si substrates, and after reduction in flowing hydrogen gas at 290°C, pure cobalt with hexagonal crystal structure and multi-branched structures were created. Anisotropic magnetic properties were found for cobalt multipods. The growth mechanism of CoO multipods will be presented in this work.

This work is supported by DOE, NSF-MRSEC, NRI and NCMN.

12:27PM P14.00007 Magnetic Exchange Force Microscopy, ALEXANDER SCHWARZ, Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — Magnetic Exchange Force Microscopy (MExFM) is a new technique that was proposed [1] to perform magnetic imaging with atomic resolution. It is based on conventional atomic force microscopy, but uses a magnetic tip, which is approached between the molecule and the substrate electrons. The different pathways for electrons lead to interference effects and generate kinks in the differential conductance at the energies for the singlet and triplet. These features are related to Fano resonance due to the branched electron wave functions. Since the ratio between the tunnelling through the two atoms can be modulated by spatial movements of the tip along the surface this suggests a technique for detection of the singlet-triplet exchange splitting with STM.

1 [R. Wiesendanger et al., J. Vac. Sci. Technol. B 9, 519 (1990).]
2 [S. Heinze et al., Science 288, 980 (2000).]
3 Support from fthe Deutsche Forschungsgemeinschaft (SFB 668) is gratefully acknowledged.

1:03PM P14.00008 Micromagnetic Modeling of Ferromagnetic Resonance in Nonuniform Magnetic Field, D.V. PELEKHOV, The Ohio State University, I. MARTIN, Los Alamos National Laboratory, YU. OBUKHOV, J. KIM, The Ohio State University, E. NAZARETSKI, Los Alamos National Laboratory, T. MEWES, The University of Alabama, P.E. WIGEN, The Ohio State University, R. MOYSHOVICH, Los Alamos National Laboratory, P.C. HAMMEL, The Ohio State University — We compare micromagnetic modeling of Ferromagnetic Resonance (FMR) excitations in thin ferromagnetic samples in the presence of a nonuniform magnetic field to our FMR data obtained with Magnetic Resonance Force Microscopy (MRFM). MRFM is a novel scanned probe technique based on mechanical detection of magnetic resonance. Its extreme sensitivity originates partially from the high magnetic field gradient of the MRFM probe micromagnet. The presence of the high field gradient imposes unusual conditions on the FMR resonance in the sample under investigation. We will discuss their manifestations in both simulations and experimental data.

1:03PM P14.00008 Micromagnetic Modeling of Ferromagnetic Resonance in Nonuniform Magnetic Field, D.V. PELEKHOV, The Ohio State University, I. MARTIN, Los Alamos National Laboratory, YU. OBUKHOV, J. KIM, The Ohio State University, E. NAZARETSKI, Los Alamos National Laboratory, T. MEWES, The University of Alabama, P.E. WIGEN, The Ohio State University, R. MOYSHOVICH, Los Alamos National Laboratory, P.C. HAMMEL, The Ohio State University — We compare micromagnetic modeling of Ferromagnetic Resonance (FMR) excitations in thin ferromagnetic samples in the presence of a nonuniform magnetic field to our FMR data obtained with Magnetic Resonance Force Microscopy (MRFM). MRFM is a novel scanned probe technique based on mechanical detection of magnetic resonance. Its extreme sensitivity originates partially from the high magnetic field gradient of the MRFM probe micromagnet. The presence of the high field gradient imposes unusual conditions on the FMR resonance in the sample under investigation. We will discuss their manifestations in both simulations and experimental data.
1:15PM P14.00009 Local investigations of 2 micrometer permalloy dot array using Magnetic resonance force microscopy, J. KIM, YU. OBUKHOV, D. PELEKHNOV, The Ohio State University, T. MEWES, University of Alabama, S. BATRA, Seagate Technologies, Pittsburgh, P.E. WIGEN, S. AN, T. GRAMILA, P.C. HAMMEL, The Ohio State University — Ferromagnetic resonance images of 2 micrometer diameter permalloy dots in an array with a center to center distance of 2.2 micrometer have been microscopically investigated at 4K using magnetic resonance force microscopy. Both local and global ferromagnetic resonance properties of the sample are observed due to the influence of the strong field immediately beneath the micromagnetic probe. Localized spectral changes reveal the dynamics of ferromagnetic resonance of a dot just underneath the tip and neighboring dots in proximity to the tip. The combination of spatial and spectral information is a promising new way to investigate magnetization dynamics using magnetic resonance force microscopy.

1:27PM P14.00010 Self-assembly of magnetic nanoparticles, JYEON KU, PHILLIP GEISSLER, Department of Chemistry, University of California, Berkeley — When a solution containing nanocrystals dries, the solute deposits onto the underlying substrate. The non-equilibrium nature of such a process, together with anisotropic interactions between nanoparticles, can drive the formation of intricate transitory patterns. In particular, we are investigating how magnetic nanocrystals can coalesce into faceted, mesoscopic domains that have been observed in experiments. We model the nanoparticles as dipolar spheres and use Monte Carlo methods to advance their arrangements in time from an initially dispersed configuration. Competition between short-ranged, isotropic van der Waals forces and long-ranged, anisotropic electrostatic forces generates diverse hybrid structures, which exhibit both imperfect close-packing and incomplete dipole alignment. We explore the structures obtained under various conditions and speculate on dynamical mechanisms of aggregation and pattern formation.

1:39PM P14.00011 FeCo Nanoparticles by Salt-Matrix Annealing, NARAYAN POUDYAL, GIRJA S. CHAUBEY, CHUAN-BING RONG, J. PING LIU, Department of Physics, University of Texas at Arlington — Preparation of monodisperse FeCo nanoparticles remains a challenge due to poor chemical stability of the nanoparticles during heat treatments. We report a novel route of preparation of monodisperse FeCo nanoparticles with controllable particle size and size distribution. CoFe₂O₄ nanoparticles were first prepared by chemical solution method via reduction of iron acetylacetonate and cobalt acetylacetonate. The as-synthesized CoFe₂O₄ nanoparticles were then mixed with NaCl powder particles and the mixtures were annealed in forming gas to form FeCo nanoparticles. Structural characterization showed that the FeCo nanoparticles obtained by salt-matrix annealing have been transformed to body-centered cubic (bcc) structure without sintering and agglomeration. The particle size can be well controlled by adjusting the synthetic parameters for CoFe₂O₄ nanoparticles. It is also found that the recovered bcc FeCo nanoparticles are stable under ambient condition. The magnetization of the FeCo nanoparticles is found to be size dependent.

1:51PM P14.00012 Static and dynamic magnetic properties of “dumbbell” and “flower” shaped Au-Fe₃Co nanoparticles, N.A. FREY, S. SRINATH, H. SRIKANTH, Department of Physics, University of South Florida, Tampa, FL 33620, CHAO WANG, SHOUHENG SUN, Department of Chemistry, Brown University, Providence, RI 02912 — We report studies of the static (DC) and dynamic (AC, RF) magnetization of chemically synthesized Au-Fe₃Co nanoparticles with dumbbell and flower shaped configurations. Dumbbell particles form with Fe₃Co₅ (18 nm) growing epitaxially on Au seed particles (4 ~ 8 nm). Multiple Fe₃Co₅ particles also can be made to grow on Au particles with flower-like cluster geometry. While measurements on dumbbell particles revealed standard signatures of superparamagnetism, the flower-like nanoparticles exhibited remarkable novel features. Two magnetic transitions are observed—one representing the blocking temperature (~88K) and the other (~48K) likely associated with freezing of surface spins. Our experiments revealed the presence of exchange bias (EB), high field irreversibility as well as training and memory effects. EB was also confirmed through RF transverse susceptibility measurements that directly probe the effective magnetic anisotropy and switching fields. Our studies demonstrate how engineering the configuration of nanoparticle clusters in a controlled manner can result in dramatically different magnetic properties.

2:03PM P14.00013 Magnetite nanoparticles with almost bulk magnetic properties: the role of the surfactant, KÁRSTEN HAMMER, PABLO GUARDIA, OSCAR IGLESIAS, AMILCAR LABARTA, UNIVERSITAT BARCELONA TEAM, ICMAM-CSIC TEAM — Uniform magnetite nanoparticles of 6, 10 and 17 nm were synthesised by thermal decomposion of an iron precursor. Oleic acid was used as surfactant. Saturation magnetization Mₛ reaches the expected value for bulk magnetite at low temperature, in contrast to results in small particle systems for which Mₛ is usually much smaller due to surface spin disorder. The coercive field for the 6 nm particles is also in agreement with that of bulk magnetite. Both results suggest that the oleic acid molecules covalently bonded to the nanoparticle surface yield a strong reduction in the surface spin disorder, such that the new O²⁻/surface ligands partially reconstruct the crystal field of the surface Fe cations, as suggested by XPS. This may be of relevance in biomedical applications to reduce the strength of the magnetic field required to obtain a high Mₛ and opens the question of whether Mₛ above the bulk value may be obtained by taking advantage of the external contribution. Work funded by Spanish NAN2004-08805-C04-02 and NAN2004-08805-C04-01, and CONSOLIDER CSD2006-12.
11:51 AM P15.00002 Fermi-Surface Evaluation of Anomalous Hall Conductivity using Wannier Interpolation

XINJIE WANG, DAVID VAN DER BILT, Rutgers University, JONATHAN YATES, IVO SOUZA, LBNL and University of California, Berkeley — Recently, Haldane showed that the non-quantized part of the intrinsic anomalous Hall conductivity (AHC) can be represented as a Fermi-surface property. The time-consuming integration of the Berry curvature over the entire Brillouin zone is thereby converted into a more efficient integral over the Fermi surface only. Here we present an ab-initio approach for computing the AHC which combines a Haldane-like strategy with Wannier interpolation of the Bloch functions. First, a conventional electronic-structure calculation is performed and maximally-localized Wannier functions are constructed by a post-processing step, in order to transform the full ab-initio problem into an "exact" tight-binding form. Second, the Brillouin zone is sampled by a large number of equally spaced parallel slices oriented normal to the total magnetization. We find the intersections of each Fermi surface sheet with every slice, organize these into a set of closed loops, and compute the Berry phase of the Bloch states as they are transported around these loops. The AHC is then just proportional to the sum of the Berry phases of all the loops on all the slices. The method is used to calculate the intrinsic AHC of Fe, Co and Ni.


12:03PM P15.00003 Spin Hall effect: from the ballistc to diffusive regime

ROKSANA GOLIZADEH-MOJARAD, SUPRIYO DATTA, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN-47906, USA — We describe a model based on the Non-Equilibrium Green’s function (NEGF) method that allows us to study the spin Hall effect continuously from the ballistic to the diffusive regime. Our numerical results show good agreement with recent experiments by Sh et al. [PRL 97, 096605 (2006)]. Analytical expressions for the spin accumulation density will also be presented that describe the numerical results very well as different parameters are varied.

12:15PM P15.00004 Berry-phase blockade in single-molecule magnets

GABRIEL GONZALEZ, MICHAEL LEVENBERGER, NanoScience Technology Center — We formulate the problem of electron transport through a single-molecule magnet (SMM) in the Coulomb blockade regime accounting for the tunneling of large spin of a SMM. We show that spin Berry phases associated with different tunneling paths. We show that in the case of incoherent spin states it is essential to place the SMM between oppositely spin-polarized source and drain leads in order to detect the spin tunneling in the stationary current, which exhibits topological zeros as a function of the transverse magnetic field.

12:27PM P15.00005 The anomalous Hall effect and Nernst effect in CuCr2Se4−xBrx: First principles studies

ZHONG FANG, YUGUI YAO, Institute of Physics, Chinese Academy of Sciences — The non-vanishing Berry curvature of Bloch states in ferromagnetic crystals with spin-orbit coupling (broken time reversal symmetry) can act as gauge field in the momentum space, which in turn affects the transport behavior of electrons in real space, and produces the fascinating phenomena in solid crystals. Typical example is the intrinsic anomalous Hall effect (IAHE). Recent progresses in this field not only deepen our understanding of the physics behind, but also enable quantitative evaluations of the effects from the parameter-free electronic structure calculations. In this presentation, the recent progresses in this field will be addressed with emphasis on the quantitative evaluations of IAHE and Nernst effect in ferromagnetic spinel CuCr2Se4−xBrx from the first-principles calculations.

12:39PM P15.00006 Chern Number effective Hamiltonian for Mn clusters in GaAs.

TOR OLOF STRANDBERG, Lund/Kalmar University, Sweden, CARLO M. CANALI, Kalmar University, Sweden, ALLAN H. MACDONALD, University of Texas at Austin, USA — Small numbers of Mn atoms can be manipulated into arbitrary spatial arrangements on the surface of GaAs by means of a novel STM atom-by-atom substitution technique, which enables the replacement of individual Ga atoms by Mn[1]. The tunnelling differential conductance over an isolated Mn atom reveals a large and broad resonance in the GaAs energy gap. For a Mn pair placed less than 1nm apart, the resonance splits into two peaks, whose spacing is thought to be related to the exchange-energy interaction between Mn ions. We report on theoretical results for the local density of states and the Mn acceptor-level splittings for a Mn dimer, based on a tight-binding model of Mn substitutions on the surface of GaAs. We compare our model with previous work which does not account for the surface. We then derive an effective quantum spin Hamiltonian for the Mn cluster, based on a Chern number theory developed recently, which includes Berry phase effects[2]. The influence of quantum fluctuations of the Mn spin orientations on the tunnelling differential conductance will be discussed. [1] D. Kitchen et al., Nature 442, 436 (2006). [2] C.M. Canali, A. Celovin and A.H. MacDonald, Phys. Rev. Lett. 91, 046805 (2003)

12:51PM P15.00007 Electron corrected Lorentz forces in solids and molecules in magnetic field

DAVIDE CERESOLI, RICCARDO MARCHETTI, SISSA and DEMOCRITOS, ERIO TOSATTI, SISSA, DEMOCRITOS and ICTP — We describe the effective Lorentz forces on the ions of a generic insulating system in a magnetic field, in the context of Born-Oppenheimer ab-initio molecular dynamics. The force on each ion includes an important contribution of electronic origin, which depends explicitly on the velocity of all other ions, and is given in terms of the Berry curvature, directly suitable for classical dynamics simulations. The formulation is valid at strong magnetic field, where a scheme for ab-initio simulations based on plane wave methods is outlined. As a simple analytical demonstration we present the dynamics of an H2 molecule in a weak field, describing the electrons approximately through Slater’s variational wavefunction.

1:03PM P15.00008 Tunneling anisotropic magnetoresistance driven by resonant surface states

ATHANASIUS CHANTIS, Theoretical Division, Los Alamos National Laboratory, KIRILL BELASHCHENKO, EVGENY TS YMBAL, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, MARK VAN SCHILFGAARDE, School of Materials, Arizona State University — Fully-relativistic first-principles calculations of the Fe(001) surface demonstrate that resonant surface [interface] states may produce sizable tunneling anisotropic magnetoresistance in magnetic tunnel junctions with a single magnetic electrode. The effect is driven by the spin-orbit coupling. It shifts the resonant surface band via the Rashba effect when the magnetization direction changes. We find that spin-flip scattering at the interface is controlled not only by the strength of the spin-orbit coupling, but depends strongly on the intrinsic width of the resonant surface states.

1:15PM P15.00009 Fully relativistic spin torques and spin currents

PETER WEINBERGER, ANDRAS VERNES, CMS, TU-Vienna, BALAZS L. GYORFFY, U-Bristol & CMS, TU-Vienna — In using the one-particle Dirac equation in the presence of an external electromagnetic field an exact equation of motion for the density of the four-component Bargmann-Wigner polarization operator $T_{\mu} = (\mathbf{T}, T_\tau)$ is presented, the various occurring terms of which can be viewed as the relativistic counterparts of ad hoc defined non-relativistic spin-currents and spin-transfer torques. Based on the properties of the Berry phase the particle and the magnetization density can be formulated in terms of a instantaneous resolvent $G(r, t')$ of the time dependent Dirac equation by means of contour integrations. The corresponding Greens function $G(\mathbf{r}, \mathbf{r}', z; t)$ can in turn be evaluated within a multiple scattering scheme by solving at each given time $t$ a "quasi-stationary" problem. In terms of this Greens function the time evolution of any single-particle density, i.e., also of $T_{\mu} = (\mathbf{T}, T_\tau)$ can be evaluated. As a first application the case of a single Fe atom is considered, for which very easily both a comparison with a time-dependent first order perturbational scheme can be given.

1Suppported by WWTF (Vienna Science and Technology Fund).
**1:27PM P15.00010 First principles theory of the current-modulated exchange bias.** PAUL HANEY, U. Texas at Austin, REMBERT DUINE, Utrecht University, ALVARO NUNEZ, Instituto de Fisica, PUCV, OLLE HEINONEN, Seagate Technology, ALLAN MACDONALD, U. Texas at Austin — Recent experiments[1] have demonstrated the influence of current on exchange-bias fields in point-contact spin-valve structures. With this motivation, we consider current induced torques in multilayer structures containing ferromagnetic, paramagnetic, and antiferromagnetic layers. Our description is based on ab initio spin-density-functional theory combined with the non-equilibrium Greens’ function formalism and direct microscopic evaluation[2] of spatially resolved torques. We find that current induced torques are generically present in both ferromagnetic and antiferromagnet layers. We theoretically demonstrate that current-induced torques in an antiferromagnetic layer that is exchange coupled to a ferromagnetic layer can alter exchange bias and discuss materials combinations in which this effect can be exploited. [1] Wei et al. cond-mat/0606462 [2] Haney et al. cond-mat/0611534

**1:39PM P15.00011 Conventional spin current in Dirac equation.** SOO YONG LEE, HYUN-WOO LEE, POSTECH — The spin current has been one of main concerns in the field of the spintronics. Recently Rashba[PRB 68, 241315 (2003)] pointed out that in certain nonmagnetic systems with the spin-orbit coupling, the conventional definition of the spin current leads to a rather strange prediction, namely a nonzero spin current should flow even without external biases. Though the nonvanishing equilibrium spin current does not violate the time reversal symmetry, it still led many scientists to reexamine the definition of the spin current. Recalling that the spin-orbit coupling arises due to the relativistic effects, we examine in this work properties of the conventionally-defined spin current for a Dirac electron subject to an electrostatic potential $V(r)$. Interestingly it is found that in this fully relativistic treatment, the equilibrium spin current vanishes for a wide class of $V(r)$ including those representing the zincblende structure and the asymmetric quantum well, which is in clear contrast with the nonvanishing equilibrium spin current obtained from some effective nonrelativistic Hamiltonians. The origin of this difference is also examined.

**1:51PM P15.00012 Markov Chain Analysis of Stochastic Micromagnetic Simulations.** S. HILL THOMPSON, Florida State University, G. BROWN, Oak Ridge National Laboratory, P.A. RIKVOLD, Florida State University — Stochastic micromagnetic simulations are employed to study the magnetization dynamics of a realistic model of an iron nanopillar in an oblique applied field at nonzero temperature. The result suggests the existence of more than one reversal path, revealed by the distribution of switching times. The dynamics are further analyzed by considering the system as an absorbing Markov chain and studying the properties of the associated transition matrix. In particular, the eigenvalue spectrum provides the time to cross the free-energy saddlepoint separating the metastable well from the equilibrium configuration. Additionally, eigenvectors from individual runs are used to determine which reversal path each simulation followed, since it is likely the switching-time distributions overlap. Along with projective dynamics, this analysis shows that the evolution of the faster mode is indicative of a relatively flat free-energy landscape, while the slower-mode dynamics are dominated by a well-defined metastable well.

**2:03PM P15.00013 Thermoinduced Magnetization in Antiferromagnetic Heisenberg Chains.** GREGORY BROWN, MARKUS EISENBACK, G. MALCOLM STOCKS, Oak Ridge National Lab — The magnetic properties of linear chains of classical three-dimensional Heisenberg spins, with antiferromagnetic nearest-neighbor exchange and uniaxial single-site anisotropy, are determined analytically and numerically to investigate the phenomenon of thermoinduced magnetization (TiM). TiM is the ferromagnetic response observed in nanoparticles of antiferromagnetic materials at low temperatures, with the ferromagnetic response turning as temperature increases. In the strong-anisotropy limit, TiM is shown analytically to result from the relaxation of individual spins away from the anisotropy axis. In the weak-anisotropy limit, it is shown numerically that TiM occurs only at temperatures low enough for long-range ordering of the entire finite chain. In the absence of anisotropy, long-range order does not occur and TiM is not observed. Both of these results present serious challenges to current theories, which describe TiM only in terms collective motions at $q=0$ and in the limit of vanishing anisotropy. This work was sponsored by the Laboratory Directed Research and Development Program of ORNL (GB, ME, GMS), and by the DOE-OS through the Offices of BasicSciences, Division of Materials Sciences and Engineering (GMS).

**Wednesday, March 7, 2007 11:15AM - 1:39PM — Session P20 DMP GMAG: Focus Session: Multiferroics and other Functional Materials — Colorado Convention Center 105**

**11:15AM P20.00001 The ferroelectric to antiferroelectric transition in multiferroic BiFe$_{1-x}$Cr$_x$O$_3$ epitaxial films.** DAE HO KIM, HO NYUNG LEE, MARIA VARELA, HANS M. CHRISTEN, Materials Science and Technology Division, Oak Ridge National Laboratory; Oak Ridge, TN — Work exploring the ferromagnetic response of epitaxial thin films has enhanced the understanding of the nature of the ferroelectricity and the weak parasitic ferromagnetism. In contrast, despite having similar structural and chemical properties as BiFeO$_3$, little is known about BiCrO$_3$, due to the difficulty of synthesizing single-phase material. We have grown high quality BiCrO$_3$ epitaxial films by pulsed laser deposition and revealed that they exhibit antiferroelectricity with an electric-field induced ferroelectric phase. This antiferroelectricity is consistent with the picture of the Bi lone pair inducing polarization in bismuth-based perovskites. Furthermore, we have grown BiFe$_{1-x}$Cr$_x$O$_3$ solid-solution epitaxial films from BiFeO$_3$ and BiCrO$_3$ targets and observed a ferroelectric to antiferroelectric transition with increasing the Cr content. The interplay between the structural and (anti) ferroelectric properties and the role of the epitaxial strain will be discussed.

1. Research sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC.

**11:27AM P20.00002 Broadband Characterization of Multiferroic Thin-Films.** NATHAN ORLOFF, JORDI MATEU, National Institute of Standards and Technology, Boulder, CO 80302, USA, MAKOTO MURAKAMI, Department of Material Science and Engineering, University of Maryland, College Park, MD 20742, USA, ICHIRO TAKEUCHI, Department of Physics, University of Maryland, College Park, MD 20742, USA, JAMES BOOTH, National Institute of Standards and Technology, Boulder, CO 80302, USA — The electromagnetic response of ferroelectric and multiferroic thin films at microwave frequencies is important for a fundamental understanding of these materials, as well for potential applications in electronics and communications systems. We explore the high-frequency response (to 40 GHz) of dielectric thin-film samples using a distributed measurement technique that utilizes patterned transmission line devices. We combine these measurements with measurements of lumped-element capacitors at lower frequencies (100 Hz - 100 MHz) to obtain true broadband measurements (100 Hz - 40 GHz) of the complex permittivity of thin film samples as a function of temperature, and electric- or magnetic-field bias.

**11:39AM P20.00003 Quantum Monte Carlo calculations of BiFeO3.** LUCAS K. WAGNER, DAVID SULOCK, LUBOS MITAS, North Carolina State University — Multiferroic Bismuth Ferrite (BiFeO3) exhibits both ferroelectricity and antiferromagnetism, possibly enabling a connection between the two effects in the same material. While its antiferromagnetic character is relatively well-understood, experimental measurements of the spontaneous polarization vary significantly over two orders of magnitude, from 0.06 C/m$^2$ to 1.90 C/m$^2$. We carry out accurate quantum Monte Carlo calculations to estimate the cohesion energy and the ferroelectric distortion well depth. We discuss the mechanisms proposed to understand the variations of polarization experimental data in the light of our quantum Monte Carlo results.

1. Funding by an NSF Graduate Research Fellowship
11:51 AM P20.00004 Ab-initio investigation of ferroelectricity in asymmetrically layered magnetic perovskites, ALISON HATT, NICOLA SPALDIN, University of California, Santa Barbara — In an effort to combine magnetism and ferroelectricity in a single material, we are motivated to explore composites in ferroelectric materials that allow the coexistence of magnetism and ferroelectricity. In this talk we present results from an ab-initio study of a system of asymmetrically layered magnetic perovskite oxides in which the asymmetric layering should induce a ferroelectric polarization. We investigate this prediction in a model system of La(Al,Fe,Cr)O$_3$, and find that a large switchable ferroelectric polarization can indeed be obtained, although it does not originate from the asymmetric layering. We examine the forces driving polarization in this system, and propose two- and three-dimensional heteroepitaxy as a general route to stabilizing novel ferroelectrics and multiferroics.

12:03PM P20.00005 Bond polarization induced by magnetic order, JUNG HOON HAN, SungKyunKwan University, CHENGLONG JIA, KIAS, SHIGEKI ŌNODA, NAOTO NAGAOA, University of Tokyo — A number of recent experimental breakthroughs have revived interest in the phenomena of coupling of magnetic and electric (dipolar) degrees of freedom in a class of materials known as “multiferroics”. Some noteworthy observations include the development of dipole moments accompanying the collinear- to- helical spin ordering and adiabatic control of dipole moments through sweeping of applied magnetic fields, which all unambiguously point to the strong coupling of electric and magnetic degrees of freedom in these compounds. A number of phenomenological and microscopic theories has been advanced to establish the connection between noncollinear spin order and ferroelectricity. In particular the work of Katsura, Nagaosa, and Balatsky proposed a microscopic theory for the interplay between non- collinear magnetic order and the dipolar polarization of the electronic wave function induced by it. The magnetic (M) ion is modeled by three degenerate $I_{23}$ levels, each carrying an external magnetic field (to guarantee magnetic order) and subject to spin-orbit coupling. Two such magnetic ions are bridged by an intermediate oxygen (O) atom which itself has no spin-orbit interaction. Solving the model Hamiltonian perturbatively in the M-O-M hybridization amplitude, KNB finds an electronic polarization orthogonal to the M-O-M axis in the ground states of one and two holes.

12:15PM P20.00006 Resonant soft x-ray scattering study of the multiferroicity in TbMn$_2$O$_5$, J. OKAMOTO, D. J. HUANG, K. S. CHAO, H.-J. LIN, C. T. CHEN, National Synchrotron Radiation Research Center, Taiwan, C. Y. MOU, National Tsing Hua University, Taiwan, S. PARK, S.-W. CHEONG, Rutgers University, USA — TbMn$_2$O$_5$ is one of the fascinating multiferroic compounds whose spontaneous polarization can be controlled by applying magnetic field. Neutron diffraction measurements reported that incommensurate-commensurate transition of antiferromagnetic ordering is related to the appearance of ferroelectricity. In order to investigate the relationship between magnetic ordering and ferroelectricity associated with electronic structures of the Mn $3d$ states, we measured soft x-ray resonant magnetic scattering of the single crystalline TbMn$_2$O$_5$ with photon energies around Mn $I_{23}$ edge. We observed that antiferromagnetic ordering of TbMn$_2$O$_5$ with incommensurate propagation vectors $(\frac{1}{2} \pm \delta_1, 0, \frac{1}{2} \pm \delta_2)$ coexists with antiferromagnetic ordering with a commensurate propagation vector $(0, 0, \frac{1}{2})$ in the ferroelectric phase ($22 K < T < 37 K$). Comparing the temperature dependence of resonant x-ray scattering and the arguments based on symmetry considerations, we discuss the magnetic ordering which leads to the magnetoelectric effect in TbMn$_2$O$_5$.

12:27PM P20.00007 Growth and Characterization of Low Loss BaM-BSTO Multilayer Films, JAYDIP DAS, ARKAJIT ROYBARMAN, CARL PATTON, Department of Physics, Colorado State University, Fort Collins, Colorado, USA, BORIS KALINIKOS, St. Petersburg Electrotechnical University, 197376, St. Petersburg, Russia — Ferrite/ferroelectric multilayer films are attractive as electronic materials because of the unique possibility of the electric field tuning of magnetic properties and vice versa. Up to now, however, it has not been possible to produce such layered structures with low microwave magnetic loss. The present work demonstrates the realization of pulse laser deposited low loss barium ferrite (BaM) in a BaM - barium strontium titanate (BSTO) layered film. The structure, from top to bottom, consists of a gold layer (30 nm), a polycrystalline BSTO layer (0.5 μm), another gold layer (30 nm), and a c-axis oriented BaM (0.5 μm) layer on a sapphire substrate. X-ray diffraction shows all components. Hysteresis loop and ferromagnetic resonance data show a low-loss behavior of a low-loss axis-orientated uniaxial BaM component. Capacitance measurements indicate a somewhat low but electric field tunable dielectric constant of the BSTO component. Supported in part by the ARO-MURI and ARO-DARPA-Seeding programs.

12:39PM P20.00008 Ferroelectric switching induced magnetic anisotropy in Fe/BaTiO$_3$ bilayers, CHUN-GANG DUAN, Department of Physics and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, S. S. JASWAL, E. Y. TS YMBAL — Ferromagnetic/ferroelectric heterostructures have recently attracted significant interest due to their potential applications in multifunctional electronic devices. We have recently measured a magnetoelastic effect at the Fe/BaTiO$_3$ interface induced by ferroelectric polarization. Preliminary results show that the ferroelectric switching of the BaTiO$_3$ has appreciable effect on the magnetic anisotropy of magnetic Fe films. This should be of interest in multiferroic device applications. [1] Chun-gang Duan, S. S. Jaswal, E. Y. Tsymbal, Phys. Rev. Lett. 97, 047201 (2006).

12:51PM P20.00009 Magneto-electric Coupling in Ferromagnetic Cobalt/Ferroelectric Copolymer Multi-layer Films, A. MARDANA, Dept. of Physics & Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, MENGIJUN BAI, University of Missouri-Columbia, A. BARUTH, S. DUCHARM, S. ADENWALLA, Dept. of Physics & Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln — We report on the magnetoelastic coupling of a thin multi-layer film sandwich consisting of ferromagnetic Cobalt (10 nm)/ferroelectric polymer (PVDF-TrFE)/ferromagnetic Cobalt (10 nm). The metallic ferromagnetic 1nm wide electrodes are deposited perpendicular to each other through a shadow mask. The ferroelectric polymer films (53nm thick) are deposited by the Langmuir-Blodgett technique. The ferromagnetic and ferroelectric layers of the samples have been characterized by the Magnetooptical Kerr Effect (MOKE) and the pyroelectric effect, respectively. Preliminary measurement results show a magneto-electric coupling is observed, with the pyroelectric reaction decreasing by ~30% on application of a 2kG field. Our observations indicate that the polarization change occurs abruptly at the closing of the magnetic hysteresis loop, shows little hysteresis and is even with magnetic field. The change is far too large to be accounted for by the magnetostriiction of Co. Possible explanations for this unexpectedly large effect are discussed. NSF Grant No MRSEC DMR-0213808

1:03PM P20.00010 Natural off-stoichiometry and asymmetry in p-n-dopability of wide-gap oxides, S. LANY, J. OSORIO-GUILLEN, H. RAEBIGER, A. ZUNGER, National Renewable Energy Lab. — Oxides such as In$_2$O$_3$ and ZnO can be doped n-type and are naturally anion deficient, while oxides such as NiO and Cu$_2$O are p-type and tend to be naturally metal-deficient. Furthermore, they exhibit the property of transparent conductivity, unlike most oxides. To decipher these phenomena, we perform thermodynamic simulations based on first-principles calculated formation energies of many neutral and charged defects. We find that the metal-vacancies (and not O-interstitials) in NiO and Cu$_2$O are responsible for their simultaneous metal deficiency and p-type conductivity. The O-deficiency of In$_2$O$_3$ and ZnO is caused by the O-vacancy VO (and not the metal interstitials). Since VO has a deep level in the gap, it does not provide for equilibrium stable n-type conductivity. We suggest, however, that a metastable state of VO in In$_2$O$_3$ and ZnO can cause persistent photoconductivity, and can explain the paradoxical coexistence of coloration (deep absorption level in the optical range) and conductivity (shallow level), which is observed after metal rich growth. By calculating the band offsets, we further show that the p-type dopability of NiO is facilitated by the relative high energy of the valence band maximum, while the n-type dopability of ZnO is facilitated by the relative low energy of the conduction band minimum.

1 Funded by DOE-BES under contract DE-AC36-99GO10337
1:15PM P20.00011 Raman scattering studies of resistance-changing NiO films with and without IrO₂ buffer layers ¹, S. YOON, E. CHO, Division of Nano Sciences and Department of Physics, Ewha Womans University, Seoul, Korea, H. CHEONG, Department of Physics, Sogang University, Seoul, Korea, S. SEO, Samsung Advanced Institute of Technology, Korea, B. SCHULZ, M. RUEH-HAUSEN, Institute of Applied Physics, University of Hamburg, Hamburg, Germany — NiO films are known to exhibit resistive memory switching behavior and inserting thin IrO₂ layers between electrodes and the NiO film is claimed to minimize the dispersion of memory switching parameters, thus greatly improving the device properties. We present Raman scattering results of a NiO film, a NiO film with a 20 nm-thick IrO₂ layer, and a NiO film with a 50 nm-thick IrO₂ layer. We discuss the microscopic structural changes in the three different films and their relations to the switching behavior changes. We also discuss the role of IrO₂ buffer layers in the device structures. ¹S. Yoon and E. Cho are supported by Korea Research Foundation Grant funded by Korea Government (MOEHRD, Basic Research Promotion Fund) (KRF-2006-331-C00099).

1:27PM P20.00012 Molecular Beam Epitaxy of MgO on Perovskite Substrates, M. SNYDER, J. XU, Engineering Science and Mechanics, Pennsylvania State University, P. FISHER, M. SKOWRONSKI, P. SALVADOR, Materials Science and Engineering, Carnegie Mellon University, O. MAKSIMOV, V. HEYDEMANN, Electro-Optics Center, Pennsylvania State University — Rock salt oxides are promising interface layer materials for the integration of multifunctional oxides with semiconductors (Si, SiC, and GaN). Although rock salt oxides were previously grown on a wide range of semiconductor (Si and GaAs) and oxide (LaAlO₃ and SrTiO₃) substrates, the influence of lattice mismatch on the crystalline quality of the films was not studied. MgO thin films were grown by molecular beam epitaxy on LSAT, LaAlO₃ and SrTiO₃ perovskite substrates to investigate the effects of lattice mismatch on the film crystal quality. Despite a lattice mismatch of ~7.9% and ~9%, respectively, epitaxial growth of MgO was achieved on SrTiO₃ and LSAT substrates. Films grown on LaAlO₃ substrates exhibited a lattice mismatch of ~10.5% were polycrystalline. yet epitaxial MgO on LaAlO₃ was deposited after the introduction of a SrTiO₃ buffer layer. The effects of deposition rate, substrate temperature, ozone flux, SrTiO₃ buffer layer thickness and stoichiometry were also investigated. This work was supported by the Office of Naval Research under grants N00014-05-1-0238 and N00014-06-1-1018.

Wednesday, March 7, 2007 11:15AM - 2:15PM — Session P24 DPOLY DMP: Focus Session: Organic Heterojunction Photovoltaics Colorado Convention Center 201

11:15AM P24.00001 Organic Semiconductors: A Molecular Picture of the Charge-Transport and Energy-Transport Processes, J. LUC BRÉDAS, Georgia Institute of Technology — Conjugated organic oligomer and polymer materials are being increasingly considered for their incorporation as the active semiconductor elements in devices such as photo-voltaic cells, light-emitting diodes, or field-effect transistors. In the operation of these devices, electron-transfer and energy-transfer processes play a key role, for instance in the form of charge transport (in the bulk or across interfaces), energy transport, charge separation, or charge recombination [1]. Here, we provide a theoretical description of electron-transfer phenomena based on electron-transfer theory, which allows us to provide a molecular, chemically-oriented understanding. In this presentation, we focus on the parameters that impact the mobility of charge carriers [2], that is the electronic coupling within chains and between adjacent chains and the reorganization energy of the chains upon ionization. Materials under study include conjugated oligomers such as oligoacenes, oligothiophenes-acenes, oligo(thiophenes) and oligo(thienoacenes) [1].


11:51AM P24.00002 Predicting structure/property relations in polymeric photovoltaic devices, GAVIN BUXTON, NIGEL CLARKE, Durham University — Plastic solar cells are attractive candidates for providing cheap, clean and renewable energy. However, such devices are critically dependent on the internal structure, or morphology, of the polymer constituents. We have developed a model that enables us to predict photovoltaic behaviour for arbitrary morphologies, which we also generate from numerical simulations. We illustrate the model by showing how diblock copolymer morphologies can be manipulated to optimise the photovoltaic effect in plastic solar cells. In this manner, we can correlate photovoltaic properties with device structure and hence guide experiments to optimise polymer morphologies to meet photovoltaic needs.

12:03PM P24.00003 Synthesis and Application of Conducting Block Copolymers in Organic Photovoltaics, BRYAN W. BOUDOURIS, MARC A. HILLMYER, C. DANIEL FRISBIE, University of Minnesota — Recent advances in the fabrication and post-processing of polymer – fullerene bulk heterojunction solar cells have allowed for devices with power conversion efficiencies up to 5% to be generated. An understanding of how the internal morphology of the active layer affects device performance would facilitate optimization and ultimately lead to higher efficiencies. Block copolymers have been shown to self-assemble into well-structured, microphase-separated domains on the order of the diffusion length (~10 nm) of an exciton (bound electron-hole pair) in thin films. In an effort to make a nanostructured active layer morphology we have synthesized block copolymers where the conducting moiety is either poly(3-hexylthiophene) or poly(3-dodecylthiophene) and the second, etchable block is polylactide. Hydroxyl-terminated polylactide molecules were synthesized via the McCullough method and used as macroinitiators for the ring-opening polymerization of D,L-lactide. AFM images of spin-coated block copolymer films show separation between the polylactide and polylactide segments. After subjecting the samples to a dilute aqueous base for short periods of time, we have selectively etched the polylactide segments to create pits in the semicrystalline polylactide matrices. In addition to these findings, preliminary device results will also be discussed.

12:15PM P24.00004 Fluorescence of Dendrons based on Donors and Acceptor with Different Linkages, J.H. PARK, Y. WU, The Ohio State Univ. Columbus, OH 43210, D.A. MODARELLI, Univ. of Akron, Akron, OH 44325, J.R. PARQUETTE, A.J. EPSTEIN, The Ohio State Univ. Columbus, OH 43210 — Earlier indirect studies utilizing wavelength and bias spectra of photocurrent in simple photovoltaic cells demonstrated charge transfer (CT) in 1st generation dendritic macromolecules prepared using two different donor (tetraphenylporphin) groups bound to an acceptor (naphthalenediimide) group. We report here fluorescence for solid-state films and solutions of these donor and dendrons. Using 460nm excitation, fluorescence (660nm, 715nm) in solution samples can be observed for both donor and dendron but fluorescence in the solid state can be observable only in donor sample due to fluorescence quenching within the dendron. This demonstrates intermolecular CT from donor to acceptor. Fluorescence lifetime measurements (460nm 1.5nsec FWHM pulse excitation) of donor and dendron solutions show that it depends on length of the linkage between donor and acceptor. This shows a direct relaxation path from donor to acceptor (intramolecular CT). The separation of the excitation to separate electron and on the donor and acceptor portions of the dendron would open the potential for its use in photovoltaic application. Supported in part by DOE #DE-FG02-01ER45931.
12:27 PM P24.00005 The interplay of morphology and carrier recombination in dendrimer-based organic photovoltaics. ∼ SEAN SHAHEEN, NIKOS KORIDAKIS, WILLIAM MITCHELL, National Renewable Energy Laboratory, WILLIAM RANCE, Dept. of Physics, Colorado School of Mines, JAO VAN DE LAGEMAAT, GARRY RUMBLES, National Renewable Energy Laboratory — Pi-conjugated dendrimers provide an alternative to polymers in organic photovoltaic devices that allow for systematic study of how the molecular structure affects the morphology of the donor and acceptor components and subsequently how the device operates. The degree of mixing and specific geometry of the donor-acceptor blend play a determining role in the rate of exciton dissociation as well as the efficacy of charge transport out of the active layer. We find that conjugated, dendritic molecules are more miscible with the fullerene-derivative acceptor than their polymeric counterparts, which leads to smaller domains than are commonly found in polymer-fullerene blends. Here we discuss how these differing morphologies affect exciton dissociation, carrier transport, and carrier recombination in the devices.

12:39 PM P24.00006 Below gap external quantum efficiency of organic solar cells. ∼ ALEXANDRE NDOBE, VALY VARDENY, University of Utah — We fabricated a variety of organic bulk hetero-junction photovoltaic (PV) solar cells based on blends of regio-regular poly(phenylene vinylene) (P3HT) and MEHPPV with the fullerene molecules C60- and C70- PCBM. We found, surprisingly, that the organic devices show a photovoltaic effect even when excited with light having photon energy below the optical gap of the polymers. This implies that organic solar cells efficiencies can be improved by considering material other than PCBM that have higher infrared absorption but still can serve as good acceptors for the polymers. To complement this finding we measured the excitation dependence of various PV parameters such as the PV fill-factor, open-circuit voltage, and external quantum efficiency. The interesting excitation spectra reveal the device structure geometry as will be discussed in detail.

12:51 PM P24.00007 Nanocrystalline organic solar cells. ∼ FAN YANG, Department of Electrical Engineering, Princeton University, KAI SUN, Electron Microbeam Analysis Laboratory, University of Michigan, Ann Arbor, STEPHEN FORREST, Departments of EECS & Physics, University of Michigan, Ann Arbor — Donor/acceptor (DA) heterointerfaces effectively dissociate excitons into carriers in organic solar cells. Unfortunately, the low carrier mobility of amorphous DA blends limits the active layer thickness to ~25 nm, resulting in low solar absorption. Solar cells made from blends of organic and inorganic semiconductor nanorods overcome the low charge mobility in disordered organic films but have disadvantages due to the mismatch between the nanorods and organic material properties. Here we demonstrate organic solar cells in which both DA materials grow into an extended nanocrystalline network. Structural analysis confirms the existence of crystalline phases of the constituent donor molecule, copper phthalocyanine (CuPc), and the acceptor, C60. The structure has a power conversion efficiency of 6.2±0.3% at 1 sun, AM1.5 simulated solar illumination. This cell shares many of the merits of all organic DA blends and organic/inorganic nanorod cells without many of their disadvantages.

1:03 PM P24.00008 Fabrication and characterization of photovoltaic devices based on 'self corralled' CdSe nanorods functionalized with polythiophene ∼ SURESH GUPTA, QINGLING ZHANG, ALI CIRPAN, FRANK KARAZ, TODD EMRICK, THOMAS P. RUSSELL, University of Massachusetts, Amherst — It has been shown that the CdSe nanorods can be oriented normal to the surface by employing an electric field and a polymer matrix where nanorods phase separate. The nanorods close pack with orientation normal to surface in a thin film when the CdSe nanorods are functionalized with alkane and poly(methyl methacrylate) or poly(3-hexyl thiophene)(P3HT) is the matrix. The film is drop cast under electric field. The phase separation of the nanorods in polymer matrix can be directed by using a patterned surface. The patterned surface was prepared by self-lithography. Further, the nanorods functionalized with P3HT are 'self corralled' under electric field by using a polymer matrix and photovoltaic devices are fabricated. The devices are characterized and the results for devices with normally oriented nanorods are compared to the devices with nanorods parallel to surface.

1:15 PM P24.00009 Femtosecond transient studies of photoinduced charge transfer in polymers doped with strong acceptor molecules; applications for organic solar cells ∼ JOSH HOLT, TOMER DRORI, University of Utah, CHUANXIANG SHENG, College of Optical Sciences, University of Arizona, Z. VALY VARDENY, University of Utah — Current developments in organic solar cells (~5% efficiency nowadays) require understanding and control of photoinduced charge carrier transfer and electronic state dynamics of donor-acceptor pairs. One current drawback to organic solar cell efficiency is negligible absorption in the near infrared region of the solar spectrum. We provide and compare evidence that poly(2-methoxy-5(2'-ethyl)hexoxy-phenylenevinylene) (MEH-PPV) and regio-regular poly-3-hexyl thiophene (RR-P3HT) doped with 2,7-dinitrofluorone (DNF) or 2,4,7-trinitrofluorenone (TNF) form below-gap charge transfer complex state that can extend absorption into the near infrared. Using fs transient and CW spectroscopies we found that the photoluminescence and mid-ir photoinduced absorption (PA) band of excitons are simultaneously quenched, when excited in the visible/uv or near ir. We compare our results to those of comparable systems using C60 as acceptor molecules.

1:27 PM P24.00010 Photoinduced charge transfer from polymers to fullerene molecules revisited. ∼ TOMER DRORI, Physics Department, University of Utah, CHUANXIANG SHENG, ALEX NDOBE, CUNG YANG, MINGHONG TANG, VALY VARDENY — We study the process of photoinduced charge transfer (PCT) between conjugated polymers and fullerene molecules as electron acceptors, using the technique of picosecond transient, and steady state photomodulation at various modulation frequencies and temperatures. The polymers studied were MEH-PPV and regio-regular P3HT [RR-P3HT], which are some of the common polymers that are used in organic photovoltaics, as well as polyfluorene [PFO] with optical gap in the blue spectral range; whereas the fullerene molecules where C60, C70 and their PCBM variations. In all cases we found PCT as evident by the formation of strong photoinduced absorption (PA) polaron bands in the mid ir spectral range. Surprisingly we also found PCT with photon energy below the polymer optical gap. This below-gap PCT process will be discussed and compared with the more usual PCT process with above gap excitation.

1:39 PM P24.00011 Nanoscale Composition and Efficiency of Conjugated Polymer Based Photovoltaic Devices ∼ BENJAMIN WATTS, North Carolina State University, CHRIS MCNEILL, Cavendish Laboratory, LARS THOMSEN, WARWICK BELCHER, The University of Newcastle, HARALD ADE, North Carolina State University, NEIL GREENHAM, Cavendish Laboratory, PAUL DASTOOR, The University of Newcastle — Organic solar cells based on thin blend films of conjugated polymers and/or fullerene derivatives promise significant advantages in flexibility and low-cost fabrication over conventional, silicon based devices. However, these polymer systems tend to display complex segregation of the component materials during film formation, with the degree of segregation observed shown to depend on parameters such as spincompeting spin-speed and solvent type. Many studies in recent years have demonstrated a link between film morphology and device performance and subsequent changes in fabrication methods have resulted in improved device efficiencies that now approach 5% total power conversion. Here, we present studies providing further details on the morphology-efficiency relationship through the application of scanning transmission X-ray Microscopy (STXM) to generate quantitative composition maps of conjugated polymer blend films and comparison to the measured efficiency of photovoltaic devices incorporating corresponding blend film active layers.

1:51 PM P24.00012 Optimization of the Negative Electrode in Organic Photovoltaic Devices ∼ MATTHEW REESE, National Renewable Energy Laboratory, MATTHEW WHITE, University of Colorado, Boulder, GARRY RUMBLES, DAVID GINLEY, SEAN SHAHEEN, National Renewable Energy Laboratory — A blend of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61-butyric acid methyl ester (PCBM) is used as the active layer in a series of bulk heterojunction organic solar cells. This polymer blend serves as a test-bed to explore the significant effects on device performance of using low work function metals and/or alkali metal halides as the top, negative electrode. Work function values reported in the literature are compared with those measured for our thin films. A series of contact materials are investigated including Al, Ca/Al, Ba/Al, LiF/Al; many devices are prepared with each contact type to validate the statistical significance of the results.
of Bulk Heterojunction Organic Photovoltaic Devices. NIKOS KOPIDAKIS, ANDREW FERGUSON, SEAN SHAHEEN, GARRY RUMBLES, National Renewable Energy Laboratory — Bulk heterojunctions composed of a blend of the polymer poly(3-hexylthiophene) (P3HT) and the acceptor fullerene derivative [6,6]-phenyl C_{61}butyric acid methyl ester (PCBM) are the prototypical organic photovoltaic devices. The photophysical processes that take place in these structures involve exciton generation and quenching, and free carrier transport, trapping and recombination. To probe these processes we have performed contactless Time-Resolved Microwave Photoconductivity measurements in pure polymer films and in bulk heterojunctions with varying PCBM concentration. We compare our results with various models for free carrier generation in the pure polymer and in the bulk heterojunction and develop a kinetic scheme to describe free carrier generation and recombination that is consistent with our experimental data. We show that exciton quenching in the presence of the acceptor (PCBM) involves first and second order processes that become prevalent at low and high light intensities, respectively.

Wednesday, March 7, 2007 11:15AM - 2:03PM —
Session P27 DMP DCOMP: Focus Session: Computational Nanoscience V - Nanotubes

11:15AM P27.00001 Absorption Coefficient for Cylindrical Nanotubes. GODFREY GUMBS, ANTONIOS BALASSIS, Hunter College/CUNY — A self-consistent field theory is presented for calculating the absorption coefficient for a pair of coaxial tubules. The spatially nonlocal dynamic formalism is obtained in terms of the electrostatic potential produced by the charge density fluctuations and the external electric field. There are peaks in the absorption spectrum arising from plasma excitations corresponding either to plasmon or particle-hole modes. We calculate numerically the plasmon contribution to the absorption. The number of peaks depends on the radius of the inner as well as outer tubule. The height of each peak depends on the plasmon wavelength and energy. For a chosen wavenumber, the most energetic plasmon has the highest peak corresponding to the largest oscillator strength. Some of the less energetic plasmon modes have such weak coupling to an external electric field that they are not seen on the same scale. We plot the peak positions of the plasmon excitations on a pair of coaxial tubules. The coupled modes on the two tubules are split by the Coulomb interaction. The energies of the two highest plasmon branches increase with the radius of the outer tubule. On the contrary, the lowest modes decrease in energy as this radius is increased.

11:27AM P27.00002 Nanocables made of a transition metal wire and boron nitride. CHIH-KAI YANG, Chang Gung University, Kueishan 333, Taiwan, ROC; JIJUN ZHAO, Dalian University of Technology, Dalian, China 116024, JIANPING LU, Department of Physics & Astronomy, University of North Carolina, Chapel Hill, NC 27599-3255 — The boron nitride (BN) nanotube has a very wide band gap and can shield the nanowire encapsulated inside its cavity from outside interference. Our calculations indicate that transition metal wires can be inserted inside a variety of zigzag BN nanotubes exothermically. In particular a cobalt wire and the BN tube interact just like two giant molecules. The weak interaction between the BN tube and the wire ensures a low binding energy and a high magnetic moment that comes solely from the transition metals. High spin polarization at the Fermi level also indicates that the hybrid structure can be used as a nanovalve for spintronic applications.

Three supported by the National Science Council of the Republic of China under grant number NSC 95-2112-M-182-001-MY3.

11:39AM P27.00003 First principles study of Crystalline Bundles of Single-Walled Boron Nanotubes. KAHR CHUN LAU, ROBERTO ORLANDO2, RAVINDRA PANDEY, Department of Physics, Michigan Technological University, Houghton, MI — First principles calculations based on density functional theory are performed to study the structural and electronic properties of the crystalline bundles of (n,0) zigzag-type single-walled boron nanotubes (SWBNT). The results predict a substantial modification in the properties of SWBNT bundles relative to those of the isolated nanotubes. The predicted modification can be attributed to a significant interplay between intra- and inter-tubular bonds in determining the stability of SWBNT bundles, analogous to the role played by intra- and inter-icosahedral bonds in the boron crystalline solids. The result shows the SWBNTs exhibit polymorphism, which is likely to be the cause of the difficulty in growing SWBNTs experimentally.

2Permanent Address: Dipartimento di Scienze e Tecnologie Avanzate, Università del Piemonte Orientale, Via Bellini 25/G, 15100 Alessandria, Italy

11:51AM P27.00004 Dielectric Response and Born Dynamic Charge of BN Nanotubes from Ab Initio Finite Electric Field Calculations. GUANG-YU GUO, Department of Physics, National Taiwan University, Taipei 106, Taiwan; SHOJI ISHIBASHI, TOMOYUKI TAMURA, Research Institute for Computational Sciences, National Institute of Industrial Science and Technology, Tsukuba, Japan, KIYOKU TAKAKURA, Creative Research Institute “Sousei”, Hokkaido University, Sapporo, Japan — Since the discovery of carbon nanotubes (CNTs) in 1991 by Iijima, carbon and other nanotubes have attracted considerable interest worldwide because of their unusual properties and also great potentials for technological applications. Though CNTs continue to attract great interest, other nanotubes such as BN nanotubes (BN-NTs) may offer different opportunities for technological applications. Currently BN-NTs attract great interest, other nanotubes such as BN nanotubes (BN-NTs) may offer different opportunities that CNTs cannot provide. In this contribution, we present the results of our recent systematic ab initio calculations of the static dielectric constant, electric polarizability, Born dynamical charge, electrostriction constant and piezoelectric constant of BN-NTs using the latest crystalline finite electric field theory.

11:03PM P27.00005 First-Principles Study of Nucleic Acid Bases Physisorbed on Graphene. S. GOWTHAM, R. H. SCHEICHER, Department of Physics and Multi-Scale Technology Institute, Michigan Technological University, Houghton, MI 49931, RAJEEN AHUJA, Department of Physics, Uppsala University, Sweden; Department of Materials Science and Engineering, Royal Institute of Technology, Sweden, RAVINDRA PANDEY, Department of Physics and Multi-Scale Technology Institute, Michigan Technological University, Houghton, MI 49931, SHASHI P. KARMA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: AMSRDL-ARM-LM, Aberdeen Proving Ground, MD 21005-5069 — We report the results of our investigation on the interaction of nucleic acid bases with graphene, carried out within the density functional theory framework, with additional calculations utilizing Hartree-Fock, more second-order Møller–Plesset perturbation theory. The calculated binding energy of the five nucleobases shows the following hierarchy: G ≈ T ≈ C ≈ A > U, though the equilibrium configuration consists of the nearly the same separation between the sheet and the bases considered. The stabilizing factor in the interaction between the nucleobases and the graphene sheet appears to be dominated by the molecular polarizability that induces a weakly attractive dispersion force between them. The present study is a first step toward understanding why different DNA sequences interact differently with CNTs, as observed experimentally.

12:15PM P27.00006 The work function of small radius carbon nanotubes. WAN-SHENG SU, TSAN-CHUEN LEUNG, Department of Physics, National Chung Cheng University, CHE-TING CHAN COLLABORATION — Carbon nanotubes workfunctions can deviate from that of graphene due to geometric and structural factors. We have systematically investigated the work functions of various forms of small radius carbon nanotubes and their derivatives by density functional calculations. We considered and compared the workfunctions of tubes and tube-bundles in order to understand the effects of chirality, tube-length and capping condition. Systematic trends are unraveled and discussed.
1:27PM P27.00007 Work function of functionalized single-wall carbon nanotubes. NICHOLAS SINGH-MILLER, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Engineering the properties of carbon nanotubes is of fundamental importance for many of their practical applications; we focus here on the work function of metallic nanotubes, and on the changes that can be induced by electrostatic or electronnegative functionalizations. We study with density functional theory pristine, hydrogenated, and fluorinated (5,5) and (5,0) nanotubes along with more complex organic ligands as functional moieties, paying particular attention to the additional dipole interactions that can arise in periodic boundary conditions. Control of the Fermi level alignment is especially relevant for field-effect devices and for the Schottky barrier at carbon nanotube interfaces.

12:39PM P27.00008 Continuum description of defects in carbon nanotubes. ELIF ERTEKIN, DARYL CHRZAN, University of California, Berkeley — Recently, indications of plastic deformation have been observed in carbon nanotubes: strain stiffening in nanotube torsional shifts and direct observations of kink motion to assist with elongation. These observations suggest the importance of defects, both their formation and dynamics, to nanotube mechanical properties. Remarkably, defect formation energies are not well-understood: formation energies of Stone-Wales defects (dislocation-like defects) vary by ≈ 3 eV, depending on the environment. Further, no attempt has been made to compute the total energies of dissociated Stone-Wales defects. To address these issues, we develop a continuum theory of defect formation in nanotubes based on the idea that the distortion field associated with the presence of a defect distribution is that which minimizes the elastic and curvature energies but is consistent with the topological constraints imposed by the defects. It makes no a priori assumptions about the defect strain fields, accounts for defect–defect interactions, and accommodates changes to the curvature and out-of-plane buckling. Formation energies of Stone-Wales defects in a wide variety of configurations are computed using total energy electronic structure methods and compared with the results of the continuum theory; the agreement is excellent, irrespective of defect arrangement. The result is an accurate and transferable continuum description of defect formation energies in carbon nanotubes.

12:51PM P27.00009 Anharmonic phonon lifetimes in graphene, graphite and carbon nanotubes. NICOLA BONINI, NICOLA MARZARI, Department of Materials Science and Engineering, MIT, Cambridge, MA, USA, MICHELE LAZZERI, FRANCESCO MAURI, Institut de Minéralogie et Physique des Milieux Condensés, Paris, France — We present a density-functional study of anharmonic phonon lifetimes in low-dimensional graphic structures. Phonon lifetimes are evaluated from the cubic terms in the interatomic potential, using density-functional perturbation theory and the 2n+1 theorem. We show that in graphene and graphite the phonon lifetimes of the E2g LO mode at Γ and the A′1 mode at K due to phonon-phonon scattering are larger than those due to the electron-phonon interaction. We discuss the relevance of this finding for the transport properties and the implications for carbon nanotubes. We also present the results for the temperature-dependent frequency shift of the Raman G mode, in which third- and fourth-order anharmonic terms contribute equally.

1:03PM P27.00010 Electronic structures of MoS2 nanotubes. LINGYUN XU, MURRAY DAW, XING GAO, ERDI BLEDA, Clemson University — The electronic structure of MoS2 nanotubes has been studied using first principles. We investigated MoS2 zigzag (n, 0) nanotubes as well as armchair (n, n) structure. We constructed MoS2 nanotube with ABA and ABC stacking. The structures have been completely optimized. We compare to previous tight-binding calculations by Seifert et al. (Phys. Rev. Lett. 85, 146 (2000)).

1:15PM P27.00011 The role of electron-phonon interactions and external strain on the electronic properties of semiconducting carbon nanotubes. DENIS KARAIKSAK, ANGELO MASCARENHAS, Center for Basic Science, National Renewable Energy Laboratory — The electron-phonon interactions play an important role in the temperature dependent photoluminescence of semiconducting carbon nanotubes. The energy shifts and spectral narrowing of the excitonic transitions can both be attributed to the electron-phonon interaction. The thermal broadening was fitted by a theoretical expression previously used to model the thermal broadening of critical points in conventional semiconductors. Moreover, careful studies of the energy shifts induced by the external strain have revealed a (n-m) family behavior. We further conclude that using a mathematical expression that combines the theory of semiconducting carbon nanotubes under hydrostatic pressure and strain, this family behavior observed experimentally could be theoretically reproduced, providing new tools to model and predict the effect of strain on the electronic properties of carbon nanotubes. The temperature dependence of the photoluminescence decay of excitons in single walled carbon nanotubes was measured for two nanotube species, (7,6) and (7,5), representative of the two nanotube (n-m)mod3 families. The effect of temperature and external strain on the photoluminescence lifetime will be discussed.


1:39PM P27.00013 Electronic structure of Defective and Deformed Single Wall Carbon Nanotubes. L.M. WOODS, YA. SHTOGUN, Department of Physics, University of South Florida, T.L. REINECKE, Naval Research Laboratory, Washinton DC — Carbon nanotube properties can be modified by the introduction of defects on their surface or by mechanical deformations. Here we present an alternative way to modify carbon nanotube characteristics by considering both types of mechanical alterations, defects and deformations, on the nanotube surface. Electronic structure calculations from first principle density functional theory using the VASP code (Vienna Ab initio Simulations Package) for metallic and semiconducting single walled carbon nanotubes with Stone-Wales defect and radial deformation are presented. The different degrees of deformation and various defect locations are analyzed in terms of the density of states and bandstructures of these systems. We compare the defective and deformed nanotube electronic structure to the electronic structure of only defective or only deformed nanotubes. In this way we determine the relative importance of the two types of mechanical alterations on the defective and deformed nanotubes.
Graphene nanostrips, and other carbon nanostructures. This work was supported by the US Office of Naval Research and the DoD HPCMO CHSSI program.

Within the framework of our computational results, we compare the band structures of graphene, single-walled nanotubes, and other carbon nanostructures. Energy gaps of the ribbons are investigated using both stability diagrams obtained at low temperatures (1.7K) and temperature dependent transport measurements at various temperatures.

First, our calculations show that the magnetic properties of nanoribbons can be controlled by electric fields. In particular, half-metallicity emerges from GNRs, a rectangular truncation of the Coulomb interaction is applied, which significantly improves the efficiency of the calculation. The quasiparticle results are compared and contrasted with results from previous studies that have been carried out either within the tight-binding or density functional formalism.
12:39PM P28.00006 Performance Limit and Scaling Behaviors of Carbon Nanoribbon Transistors, JING GUO, YUJIN OUYANG, Dept. of ECE, University of Florida — Carbon-based nanostructures promise near ballistic transport and are being intensively explored for device applications. In this work, the performance limits of carbon nanoribbon (CNR) field-effect transistors (FETs) are assessed using a semiclassical model, and compare to those of carbon nanotube (CNT) FETs. The ballistic channel conductance and the quantum capacitance of the CNRFET are about a factor of 2 smaller than those of the CNTFET, because of the different valley degeneracy factors for CNTs and CNRs. The intrinsic speed of the CNRFET is faster due to a larger average carrier injection velocity. The gate capacitance plays an important role in determining which transistor delivers a larger on-current. The scaling behaviors of CNRFETs are studied using an atomistic quantum simulation.

12:51PM P28.00007 Applications of Nanoribbon Devices, THUSHARI JAYASEKERA, JOHN W. MINTMIRE, Oklahoma State University, Stillwater, OK, USA — Modern experiments allow us to grow ultra-thin epitaxial graphene which shows two-dimensional electron gas (2DEG) behavior. Electron transport in the 2DEG systems can be efficiently controlled in lateral directions using micro-electronics lithography methods (nano-patterned epitaxial graphene, NPEG). We study the properties of the NPEG multi-terminal devices made at a crossing of a zig-zag and armchair nanoribbons, in particular, plus junction and T-junction devices. We investigate the effect of size, shape, and, chirality on the transport properties of the device. We also discuss the effect of defects in the junction region on the electron transport of the device. Our results find that the properties of nanoribbon junctions are highly sensitive to the details of the junction region, thus we can engineer different properties by changing those details of the device. This work was supported by the DoD HPCCO CHSSI program through the Naval Research Laboratory.

1:03PM P28.00008 Ballistic transport in zigzag-edge graphene nanostrips, DANIEL GUNLYCKE, Naval Research Laboratory, HADLEY M. LAWLER, University of Washington, DENIS A. ARESHKIN, George Washington University, CARTER T. WHITE, Naval Research Laboratory — Graphene nanostrips (GNSs) constitute a class of materials where one of the two in-plane dimensions of graphene has a small finite width. We present results of zigzag-edge GNSs terminated with hydrogen atoms which suggest that ballistic transport may be possible over micrometer lengths. The single channel near the Fermi level appears to possess a natural resistance to back-scattering. Long-range disorder have a negligible back-scattering since the only allowed coupling requires a large crystal momentum change. We find that disorder on atomic scale and edge disorder have also little impact on the conductance in the single-channel window. Not only are the zigzag-edge GNSs resistant to static disorder, they may also offer longer electron-phonon mean-free paths which are longer than those in carbon nanotubes. Back-scattering in the conduction band requires a large transfer of crystal momentum from phonons which immediately eliminate long-wavelength acoustic phonon scattering. Therefore, it might be feasible to have single-channel ballistic transport in zigzag-edge GNSs at room temperature.

1:15PM P28.00009 first-principles tight-binding study of band gaps in graphene ribbons, DANIEL FINKENSTADT, Naval Research Laboratory, GARY PENNINGTON, University of Maryland, CHRIS ASHMAN, HPTI, MIKE MEHL, Naval Research Laboratory — Graphene has recently received much attention for the many interesting physical properties that it exhibits, including light Dirac fermion characteristics of its charge carriers and some experimental evidence of a minimum conductivity in some of the nanoscale devices. In this work, we use the NRL tight-binding method, which is fit to first-principles calculated data, to study the possibility of opening a gap in graphene by varying strip-width, edge shape with and without termination, and by allowing Peierl’s distortion of the edges for narrow ribbons. We compare the tight-binding results with calculations based on the density functional theory.

1:27PM P28.00010 Effects of disorder in the biased graphene bilayer, JOHAN NILSSON, ANTONIO CASTRO NETO, Boston University — We discuss the effects of disorder on the peculiar electronic properties of a biased graphene bilayer, which is a semiconductor that has the property that its band-gap can be controlled externally by the field effect. We focus on the low-energy region inside of and near the band-gap and have studied the properties of bound states as well as possible effects due to a finite density of impurities such as impurity band formation and band gap renormalization.

1:39PM P28.00011 Edge disorder in armchair-edge graphene nanostrips, DENIS A. ARESHKIN, George Washington University, DANIEL GUNLYCKE, CARTER T. WHITE, Naval Research Laboratory — Graphene nanostrips created using current lithography techniques will likely contain edge irregularities due to lack of atomic precision. We present tight-binding calculations which show that these edge irregularities have a strong effect on electron transport in armchair-edge graphene nanostrips. The edge disorder causes Anderson localization which effectively suppresses the electronic conductance in samples which are longer than the mean-free path. We estimate the mean-free path via the localization length which is calculated by averaging over a large number of disordered nanostrips. We find that the localization length approximately decreases with the square of the width of the nanostrip and is of the order of tens of nanometers at the width 20 nm. The localization length also depends on the concentration of edge defects and energy. Only nanostrips with low concentration of edge disorder reflect expected semiconducting gaps in the localization length. We also find that the Anderson localization extends over the entire π-electron energy range. With this result in mind, we predict that long and narrow armchair-edge graphene nanostrips are insulators.

3This work was supported by the NRC and the ONR through the Naval Research Laboratory.

1:51PM P28.00012 Carrier transport in 2D graphene layers near the Dirac point, SHAFFIQUE ADAM, E.H. HWANG, S. DAS SARMA, Condensed Matter Theory Center, University of Maryland, College Park, MD 20742-4111, USA — In a recent work we studied carrier transport in gated 2D graphene monolayers theoretically in the presence of scattering by random charged impurity centers using a Boltzmann theory formalism (cond-mat/0610157). Comparing our results with available experimental data suggested that the low density saturation of conductivity arises from charged impurity induced inhomogeneity in the graphene carrier density. In the present work, we develop a model for carrier transport in a disorder-induced inhomogeneous potential and examine the consequences on conductivity. This work was partially supported by U.S. ONR.

2:03PM P28.00013 Dislocation and pentagon-heptagon pair generation in vacancy-induced graphene layer, BYOYOUNG WOOK JEONG, HOONKYUNG LEE, Department of Physics and Astronomy, Seoul National University, GUN-DO LEE, Department of Materials Science and Engineering, Seoul National University, JISOOK IHH, Department of Physics and Astronomy, Seoul National University — We investigate the mechanism of the generation of long range order defects in graphene layer by tight binding molecular dynamics simulations and first-principles total energy methods. It is found that the vacancies are diffused and coalesced to make the dislocation defect with the two 5-7 pair defects when more than a certain number of vacancies are present. We examine the magic number of the vacancy which gives dislocation defects in a graphene layer. STM simulation results related to the graphite lattice with the period of $\sqrt{3} \times \sqrt{3}$ in an STM topograp will be discussed.
11:15AM P39.00001 Hydrogen Storage in Chemically Reducible Microporous Ti Oxides

DAVID ANTONELLI, University of Windsor — Micro- and mesoporous Ti oxides with controlled pore sizes from 12 Å to 26 Å were synthesized. The hydrogen storage capacity at 77 K was tested as a function of surface area, pore size, and reducing agent. Surprisingly, the oxidation state of the surface Ti species had a greater effect on the storage densities than surface area or pore size. The 12 Å material reduced with bis(toluene) Ti possesses a surface area of less than 500 m²/g, but absorbs over 5 wt% and 40 kg/m³ of H₂ reversibly at 77K and 100 atm. The H₂ binding enthalpies increased from less than 5 kJ/mol to over 8 kJ/mol as the surface oxidation state of the Ti decreased. The enthalpies also increased with surface coverage, which is opposite to all other cryogenic physisorption systems. These results suggest that a Kubas-type π H₂ complex is involved and that further tuning of the H₂ binding enthalpies through use of various chemical reagents may achieve even higher storage levels at more moderate temperatures.

11:51AM P39.00002 Novel nanostructured materials with binding “pockets” for hydrogen storage media

SUNGJONG WOO, YOUNG-KYUN KWON, Dep. of Physics, Univ. of Mass. Lowell — Hydrogen storage issue is one of the key barriers to the effort to substitute the hydrogen with the conventional fossil fuel. Chemisorption using metal hydrides and physisorption using nanostructured carbon-based materials have suffered several serious problems such as low storage capacity, insufficient binding energy and poor releasing process. In order to overcome such issues, we have investigated novel nanostructured materials of low density that bear hydrogen binding “pockets”, which can significantly enhance molecular hydrogen binding – physisorption – compared to carbon-based materials. Using numerical simulation based on the density functional theory, the hydrogen-molecule binding-energies of different candidate materials are calculated and optimized. With the obtained binding energies, we develop nanostructures similar to metal-oxide-framework that maximize the hydrogen capacity of the storage. The statistical properties of the structure, which is necessary to understand the process and efficiency of hydrogen release, are studied. In order to enhance the capacity even further, we synthesize the nanostructure with transition metals and the result will be discussed.

1 Nanomannufacturing Center of Excellence and Center for High-rate Nanomannufacturing

12:03PM P39.00003 ABSTRACT WITHDRAWN

12:15PM P39.00004 Transition Metal-Ethylene Complexes as High-Capacity Hydrogen Storage Media

E. DURGUN, S. CIRACI, Physics Department, Bilkent University, Ankara Turkey, W. ZHOU, TANER YILDIRIM, NIST Center for Neutron Research and University of Pennsylvania — From first-principles calculations, we predict that a single ethylene molecule can form a stable complex with two transition metals (TM) such as Ti. The resulting TM-ethylene complex then absorbs up to ten hydrogen molecules, reaching to gravimetric storage capacity of 16 wt%. Dimerization, polymerizations and incorporation of the TM-ethylene complexes in nanoporous carbon materials have been also discussed. Our results are quite remarkable and open a new approach to high-capacity hydrogen storage materials discovery.

12:27PM P39.00005 ABSTRACT WITHDRAWN

12:39PM P39.00006 Functionalized Carbon Nanostructures as Potential Hydrogen Storage Media

MINA YOON, The University of Tennessee, Oak Ridge National Laboratory, SHENYUAN YANG, The University of Tennessee, Chinese Academy of Sciences, ENGE WANG, Chinese Academy of Sciences, ZHENYU ZHANG, Oak Ridge National Laboratory, The University of Tennessee — Nanoscaled carbon materials have attracted great attention as promising hydrogen storage media due to their light weight and high surface areas. However, a major limitation is the poor hydrogen uptake resulting from the weak interactions of hydrogen molecules with pristine carbon nanostructures. Recent theoretical studies have investigated ways to increase the binding strength of molecular hydrogen by coating and/or substitutional doping of the carbon nanostructures with transition metals, yet experimentalization of these approaches have been difficult because of metal clustering. In this talk, we study hydrogen storage in carbon nanotubes and fullerenes, by functionalizing such structures with tunable charge states. The tunability is achieved via chemical or electron doping. Our study shows that with the proper method of charge doping, the hydrogen binding strength can be substantially increased. In this way, hydrogen uptake of > 6.0 wt % at ambient conditions can be realized.

1 Supported by The BES program of USDOE, USNSF, & CAS.

12:51PM P39.00007 Theoretical study of hydrogen bonding to metal-coated carbon nanotubes

JEONGNIM KIM, University of Illinois, Urbana-Champaign, QMPCPACK DEVELOPERS TEAM — Dihydrogen transition metal complexes and carbon nanostructures are promising hydrogen storage materials [1]. While the practical storage capacity of pure carbon nanostructures is low, calculations predict a possible hydrogen capacity of above 6 wt.% for Ti coated nanotubes [2]. A unique hybridization of Ti-d, H-H σ and carbon π-orbitals was attributed for the bonding; light alkali and alkaline metals were excluded as alternatives to Ti [2]. This is at odd with earlier predictions of non-transition-metal complexes and synthesis of alkali-doped carbon nanotubes (CNT) [1]. Quantum Monte Carlo (QMC) methods are well suited to describe the strong correlation effects tha to the weak hydrogen binding and metal-hydrogen interactions. We present QMC study of hydrogen bonding to metal-coated CNT using correlated umbrella samplings. Specifically, we study hydrogen bonding to Ti and Mg at various doping levels on CNT.


1 Supported by NSF and computational support from NCSA.

1:03PM P39.00008 Interaction of Transition Metals with Carbon Nanostructures

SHENYUAN YANG, International Center for Quantum Structures and Institute of Physics, Chinese Academy of Sciences, The University of Tennessee, MINA YOON, The University of Tennessee, Oak Ridge National Laboratory, ENGE WANG, International Center for Quantum Structures and Institute of Physics, Chinese Academy of Sciences, ZHENYU ZHANG, Oak Ridge National Laboratory, The University of Tennessee — Recent theoretical studies have shown that transition-metal (TM) decorated carbon nanotubes and fullerenes may serve as promising media for hydrogen storage. However, one prerequisite for this functionality is that the metal atoms decorate the carbon nanostructures as a homogeneous layer. To date, no experimental evidence supports this feasibility; instead, several subsequent studies indicated strong preference of clustering by the TM atoms. In this talk, we investigate several possible ways to prevent TM clustering on the surfaces of carbon nanostructures, based on first-principles total energy calculations. First, we discuss the energetics and kinetics of various TMs as they interact with carbon nanostructures. We then explore the possibility to suppress or enhance clustering by electron or chemical doping.

1 Supported by CAS, The BES program of USDOE, & USNSF.
1:15PM P39.00009 First principles study of Interaction of H2 with doped Carbon Nanotube and Graphite Surfaces, LI CHEN, YIMING ZHANG, NIHIKL KORATKAR, PURU JENA, SAROJ NAYAK, RENSSELAER POLYTECHNIC INSTITUTE TEAM, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION — Using first principles density functional theory based on parameter corrected approach we have studied interaction of H2 molecule with doped carbon nanotube and graphite surfaces. In agreement with earlier study we find that H2 physisors on carbon nanotube and graphite surfaces while the binding increases dramatically when H2 binds to Li atoms decorated on carbon nanotube surfaces: the binding further enhances with Li atoms on fullerene doped nanotube peapod structures. The increase in binding in the latter structures arises due to charge transfer between the nanotube and dopants and the bonding is primarily electrostatic in nature. The bonding is further improved with decrease in diameter of nanotube suggesting a combination of various effects could be exploited for engineering suitable graphitic surfaces for molecular hydrogen storage.

1:27PM P39.00010 Endohedral Metallofullerenes: A Smart Material for Hydrogen Storage, YUFENG ZHAO, MICHAEL J. HEBEN, ANNE C. DILLON, LIN SIMPSON, JEFF BLACKBURN, National Renewable Energy Lab., HARRY C. DORN, Virginia Polytechnic Institute and State University, SHENGBAI B. ZHANG, National Renewable Energy Lab. — We report a first-principle computational study on tunable hydrogenation of the fullerene C_{60} and endohedral metallofullerenes M@C_{60} and M_{2}@C_{60} (M = Li, Be, Mg, Ca, Al, and Sc). The interaction between the encapsulated metal atoms and the C_{60} cage leads to a smart-material behavior, which tunes the hydrogen binding in a desired manner as the hydrogenation proceeds. At lower H densities, when H atoms are too strongly bound to pure C_{60}, the endohedral dopants weaken the binding. The dopants also enhance the hydrogen binding energy at higher coverages, and enable the degree of hydrogenation to be substantially increased relative to that available with un-modified C_{60}. Overall, the encapsulated metals increase the capacity and improve the energy efficiency for hydrogen storage in hydroendofullerenes.

1:39PM P39.00011 Computational Study of hydrogen storage characteristics of the Covalent-Bonded Graphites, NOEJUNG PARK, Dankook University, Seoul, Korea, SEUNG-HOON JHI, KYUBONG KIM, Pohang University of Science and Technology, Korea, SULKYUN HONG, Sejong University, Seoul, Korea — We perform electronic structure calculations to investigate hydrogen-storage characteristics of the solid carbon structures which consist of covalent-bonded graphenes. First, we show that some regular or irregular combinations of sp²- and sp³-bonded carbon atoms lead to very stable porous carbon structures, which is designated as the covalent-bonded graphites (CBGs). Using the density-functional calculation and the Muller-Plesset perturbation method we show that the H₂ molecular bindings in CBGs are stronger than those on the isolated graphene by about 20%. We also suggest the CBGs with appropriate pore sizes can be utilized as framework structures for dispersing metal atoms. Energetics show that the Ti atoms are likely to be adsorbed at vertex sites of the CBGs. The hydrogen adsorption properties on metal atoms dispersed inside the CBGs are also presented.

1:51PM P39.00012 Recombination pathways for atomic hydrogen on the graphite (0001) and single-wall carbon nanotubes, ZELIKO SLJIVANCANIN, Institut Romand de Recherche Numerique en Physique des Materiaux (IRRMA), CH-1015 Lausanne, Switzerland, LIV HORNKAER, EVA RAULIS, BJORK HAMMER, Department of Physics and Astronomy, Aarhus University, Ny Munkegade bygn. 520, 8000 Aarhus C, Denmark — Using density functional theory we investigated the lowest energy configurations of two H atoms on a graphite surface, and found two states with an approximately identical binding energy. These states are the dimer A state with two hydrogen atoms adsorbed on two neighbor carbon atoms and the dimer B state with two hydrogen atoms adsorbed on carbon atoms at opposite sides of a carbon hexagon. Hydrogen atoms in the dimer A state will recombine via diffusion into state B and then directly recombine from B. We also studied the corresponding pathways for molecular hydrogen formation from H atoms adsorbed at the single-wall carbon nanotubes and compared results to those obtained for the graphite surface.

2:03PM P39.00013 Hydrogen generation and storage over transition metal-decorated fullerenes and related materials, LIPING HUANG, Department of Chemical and Biomolecular Engineering, North Carolina State University, ERIK SANTISO, KEITH GUBBINS, Department of Chemical and Biomolecular Engineering, North Carolina State University, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University; CSMD, Oak Ridge National Laboratory — Economical ways to generate and store hydrogen are crucial steps towards the hydrogen economy and fuel-cell technologies. By using first-principles density functional theory calculations, we found out that transition metal-decorated fullerenes and related materials can simultaneously dissociate small molecules like water to produce and store hydrogen. Hydrogen production from water will allow us to have a clean hydrogen economy by using renewable source rather than fossil fuels so that we can stop releasing carbon into the atmosphere. Our studies show that the Ti atoms are likely to be adsorbed at vertex sites of the CBGs. The hydrogen adsorption properties on metal atoms dispersed inside the CBGs are also presented.

Wednesday, March 7, 2007 11:15AM - 2:03PM –
Session P42 DMP: Focus Session: Biological and Chemical Self-Assembly at Surfaces
Colorado Convention Center 505

11:15AM P42.00001 Directing the assembly of nanostructured films with living cells, C. JEFFREY BRINKER, Fellow, Sandia National Laboratories; Regents Professor of Chemical Engineering, the University of New Mexico, Albuquerque, NM. — This talk describes our recent discovery of the ability of living cells to organize extended nanostructures and nano-objects in a manner that creates a unique, highly biocompatible nano/bio interface (Science 313, 337-340, 2006). We find that, using short chain phospholipids to direct the formation of thin film silica mesophases during evaporation-induced self-assembly, the introduction of cells (so far yeast and bacteria) alters profoundly the inorganic self-assembly pathway. Cells actively organize around themselves an ordered, multilayered lipid-membrane that interfaces coherently with a lipid-templated silica mesophase. This bio/nano interface is unique in that it withstands drying (even evaporation) without cracking or the development of tensile stresses – yet it maintains accessibility to charge transfer between the nanotube and dopants and the bonding is primarily electrostatic in nature. The bonding is further improved with decrease in diameter of nanotube suggesting a combination of various effects could be exploited for engineering suitable graphitic surfaces for molecular hydrogen storage.

11:51AM P42.00002 ABSTRACT WITHDRAWN –
12:03PM P42.00003 STM studies of the molecular-level organization of chiral tartaric acid domains on Ag(111), NANCY SANTAGATA, AMIT LAKHANI, DARRYL DEVITT, THOMAS PEARL, North Carolina State University — The expression of chirality in molecular domains on surfaces has important implications for enantioselective catalysis and chemically tuned thin films. In this talk we will discuss the organizational structure of a chiral molecule, tartaric acid (C4H6O6), weakly bound to an achiral metal surface, Ag(111), as studied with low temperature scanning tunneling microscopy (STM). Molecularly resolved images of both (R, R)- and (S, S)- tartaric acid on Ag(111) will be presented, and the role of intermolecular hydrogen bonding in stereospecific domain and superlattice formation will be addressed. In addition, we will consider chiral domain formation and phase separation from a racemic mixture of both tartaric acid enantiomers. Finally, we will present data that indicates a proposed multilayer structure and discuss the growth mode associated with its formation.

12:15PM P42.00004 Inter- and intramolecular dispersion in a highly ordered organic molecular crystal. STEPHEN BERKEBILE, KF University, 8010 Graz, Austria, PETER PUSCHNIG, Montan University, Leoben, Austria, GEORG KOLLER, FALKO P. NETZER, MICHAEL G. RAMSEY, KF University, 8010 Graz, Austria — The inter- and intramolecular dispersion in organic molecular crystals have been predicted by theory, but never measured to a satisfying degree. Further, organic pi-conjugated molecules, as they are intrinsically one-dimensional objects with a well-defined number of repeating units, serve as a simple model for understanding what happens to the basic electronic structure in systems of limited size and low dimensions. Here, the band structure of a highly ordered and crystalline para-sexiphenyl (6P) film has been measured using angle-resolved photoemission spectroscopy (ARUPS) in the three directions important to charge transport in organic devices. The ARUPS behavior reveals both strong intermolecular dispersion perpendicular to the molecular axis and intramolecular dispersion along the axis of the molecules. The data will be shown to be in very good agreement with calculations in terms of the extent of the band dispersion, the ARUPS intensity and the k-spread of the peaks associated with quantum size effects.

1 supported by the Austrian Science Fund (FWF).

12:27PM P42.00005 Kinetics-driven growth mechanism of self-organized pentacene thin films, ABDULLAH AL-MAHBOOB, JERZY S. SADOWSKI, YASUNORI FUJIKAWA, KAZUO NAKAJIMA, TOSHIRO SAKURAI, Institute for Materials Research, Tohoku University, Sendai, Japan — The growth kinetics of self-organized, highly ordered (001)-oriented pentacene (Pn) thin films was studied in situ by low-energy electron microscopy (LEEM) and complementary density functional theory calculations. We propose a model of ‘molecule incorporation-controlled’ growth mechanism, according to which the attachment pathway at the island edge and the attachment energy of crystallization unit, rather than step or surface energies, determine the island shape in the kinetic growth of organic molecular thin film. We have found that experimentally observed growth anisotropy can be reproduced exactly by our model, if molecule attachment at island-edge is realized in the form of herringbone pair, for all low-indexed growth directions of Pn. P. NETZER, MICHAEL G. RAMSEY, KF University, 8010 Graz, Austria — The inter- and intramolecular dispersion in organic molecular crystals have been predicted by theory, but never measured to a satisfying degree. Further, organic pi-conjugated molecules, as they are intrinsically one-dimensional objects with a well-defined number of repeating units, serve as a simple model for understanding what happens to the basic electronic structure in systems of limited size and low dimensions. Here, the band structure of a highly ordered and crystalline para-sexiphenyl (6P) film has been measured using angle-resolved photoemission spectroscopy (ARUPS) in the three directions important to charge transport in organic devices. The ARUPS behavior reveals both strong intermolecular dispersion perpendicular to the molecular axis and intramolecular dispersion along the axis of the molecules. The data will be shown to be in very good agreement with calculations in terms of the extent of the band dispersion, the ARUPS intensity and the k-spread of the peaks associated with quantum size effects.

1 supported by the Austrian Science Fund (FWF).

12:39PM P42.00006 Improved Molecular Dynamics simulations of hexane on graphite near monolayer completion, M.W. ROTH, M.J. CONNOLLY, University of Northern Iowa, CARLOS WEXLER, University of Missouri - Columbia, PAUL A. GRAY, University of Northern Iowa — We present the results of computer simulations of hexane on graphite near monolayer completion utilizing NAMD Scalable Molecular Dynamics in parallel computing environments. We include hydrogens explicitly on the hexane molecules, and the graphite substrate is represented as six all-atom graphene sheets. Results presented for temperatures between T = 100 K and T = 200 K have features which differ from those obtained using the united Atom (UA) model, where hydrogens are suppressed. Various structural and thermodynamic quantities show that the improvement obtained from explicitly including hydrogens come not only from their interaction with the substrate but also by their manipulation of in-plane space.

1 We gratefully acknowledge support from Petroleum Research Fund grant PRF43277-B5

12:51PM P42.00007 Nucleation and post-growth relaxation of tetracene thin films on silicon oxide, JUN SHI, X. R. QIN, University of Guelph — We demonstrate that layered morphology of tetracene films on silicon oxide can be achieved at room temperature via vacuum evaporation. Island size distribution analysis shows that tetracene nucleation in a high-flux growth regime is diffusion-mediated with a critical island size i1 = 3, similar to that in pentacene growth. A pronounced post-growth relaxation has been observed on a time scale of minutes. It is suggested that the high flux rate is crucial in the growth kinetics of forming the layered morphology and also important in overcoming the effect of post-growth relaxation which is sensitive to the film coverage and substrates.

1 Supported by Natural Science and Engineering Research Council of Canada (NSERC), and Canada Foundation for Innovation (CFI) and Ontario Innovation Trust (OIT).

1:03PM P42.00008 Designing Self-assembled Nanostructures: Metal – Organic Molecule Coordination Networks at Surfaces, STEVEN L. TAIT, A. LANGNER, N. LIN, S. STEPANOW, Max Planck Institute for Solid State Research (MPI), C. RAJADURAI, M. RUBEN, Forschungszentrum Karlsruhe, Germany, K. KERN, MPI, Stuttgart, Germany — Networks of isolated metal atoms and organic ligands can be designed to self-assemble at surfaces in desired patterns, producing regular 2D nanopore lattices, whose dimensions and properties can be controlled by selection of the organic ligand. We constructed such a network by coordination of molecules containing pyridyl groups with the inherent adatom population on a Cu(100) surface at room temperature. We produced the same network on Ag(100) and Ag(111) by depositing Cu atoms with molecules, showing the network fidelity on different substrates. Rectangular networks with higher complexity were formed from two species of organic ligands with metal atom nodes. The nanopore size and aspect ratio can be tuned independently selecting the two ligand species. Some properties of these designed nanostructures can be "tuned" by rational selection of the organic molecule and metal components. We have especially explored the organic adsorption of simple molecules on these networks, which may be of interest for future chemical or catalytic applications. The ability to tailor the size and functionality of nanometer-scale arrays produced by self assembly represents a unique opportunity for molecular recognition, heterogeneous catalysis, and other fields.

1:15PM P42.00009 Real-Time Monitoring of Organic Thin Film Morphology by Organic Vapor Phase Deposition, RICHARD R. LUNT, JAY B. BENZIGER, Department of Chemical Engineering, Princeton University, Princeton, NJ, STEPHEN R. FORREST, Departments of Electrical Engineering and Computer Science and Physics, University of Michigan, Ann Arbor, MI — We demonstrate the real-time monitoring of the development of crystalline structure in the growth of films by organic vapor-phase deposition (OVPD) using high-pressure reflection high-energy electron diffraction (HP-RHEED). Through control of the probe electron beam energy, sample damage from impinging electrons was avoided and beam attenuation in the 8mTorr OVPD deposition environment was minimized. The growth of copper phthalocyanine (CuPc) on highly oriented pyrolytic graphite was used to demonstrate the ability of such in-situ organic-growth monitoring, where it was observed that the first several monolayers formed ordered films independent of the substrate temperature and deposition rate, while the evolution of thicker films was strongly affected by substrate temperature. Higher temperatures resulted in greater in-plane crystalline ordering. We thereby have shown HP-RHEED to be a powerful tool for real-time monitoring of growth morphology, ultimately leading to in-situ control of thin film crystal structure order.
1:27PM P42.00010 Characterizing the copper-based catalyst for the oxygen-assisted water-gas shift reaction at a sub-nano scale. ALOYSIUS SOON, MIRA TODOROVA, CATHERINE STAMPFL, School of Physics, University of Sydney, Australia, BERNARD DELLEY, Paul-Scherrer-Institut (PSI) — To obtain insight into the structure and surface stoichiometry of copper-beam catalysts in commercially important chemical reactions such as the oxygen-assisted water-gas shift reaction, we perform density-functional theory calculations to investigate the stability of oxide surfaces. Taking into account the pressure and temperature through the framework of ab initio thermodynamics, we identify two low energy surface structures that are most stable under such conditions which could be catalytically relevant. These oxide surface structures are found to be non-stoichiometric (with surface defects) and exhibit a metallic character. [1] A. Soon, M. Todorova, B. Delley and C. Stampfl, Phys. Rev. B 73, 165424 (2006). [2] C. Stampfl, Catal. Today 105, 17 (2005). [3] A. Soon, M. Todorova, B. Delley, and C. Stampfl, submitted to Phys. Rev. B.

1:39PM P42.00011 First-principles study of the self-organization mechanism of NH₃ on Si(001). YONG-SUNG KIM, HANCHUL KIM, Korea Research Institute of Standards and Science — We have investigated the self-organization of NH₃ molecules on the Si(001) surface using the first-principles pseudopotential calculations. In order to find out the adsorption pathways and understand the mechanism of self-organization, we have calculated the potential energy surfaces of an incoming NH₃ molecule with one pre-adsorbed NH₃ molecule. Based on the results, we propose a kinetic process model of NH₃ self-organization: (i) the incoming molecules are attracted towards the pre-adsorbed molecules due to the H-bonding interaction. (ii) By forming the H-bond with the pre-adsorbed molecule, an incoming molecule can achieve physisorption states. (iii) Subsequently, the physisorbed NH₃ molecule is attracted to adjacent “down” Si atoms to complete the molecular adsorption process. (iv) Finally, the adsorbed NH₃ dissociates into NH₂ and H fragments. The resultant self-organized pattern is in accordance with recent STM experiments. However, it is in stark contrast with the energetically favored pattern that is characterized by H-bond formation between the dissociated fragments. This indicates that the self-organization of NH₃ on Si(001) is governed by the kinetics rather than the energetics. [1] This work is supported by KISTI under “The 8th Strategic Supercomputing Support Program.”

1:51PM P42.00012 Structure of tetracene films on hydrogen-passivated Si(001) studied via STM, AFM and NEXAFS. ANDREW TERSIGNI, JUN SHI, D. T. JIANG, X. R. QIN, University of Guelph — Scanning tunneling microscopy (STM), atomic force microscopy (AFM) and near-edge x-ray absorption fine structure (NEXAFS) have been used to study the structure of tetracene films on hydrogen-passivated Si(001). STM imaging of the films with nominal thickness of three monolayers (3 ML) exhibits the characteristic “herringbone” molecular packing known from the bulk crystalline tetracene, showing standing molecules on the ab-plane. The dimensions and orientation of the herringbone lattice indicate a commensurate structural relationship between the lattice and the crystalline substrate. The corresponding AFM images illustrate that at and above the second layer of the films, the islands are anisotropic, in contrast with the submonolayer fractals, with two preferred growth directions appearing orthogonal to each other. The polarization dependent NEXAFS measurements indicate that the average molecular tilting angle with respect to the surface first increases with the film thickness up to 3 ML, then stabilizes at a value close to the bulk tetracene case afterwards. The combined results indicate a distinct growth morphological change that occurs around a few monolayers of thickness. [1] Phys. Rev. B (in press). Supported by NSERC of Canada, and Canada Foundation for Innovation (CFI) and Ontario Innovation Trust (OIT).

Wednesday, March 7, 2007 11:15AM - 2:03PM –
Session P43 DMP: Focus Session: Materials for Quantum Information Processing III Colorado Convention Center 506

11:15AM P43.00001 Complete stabilization and improvement of the characteristics of tunnel junctions by thermal annealing. ILARI MAASILTA, PANU KOPPINEN, LASSE VAISTO, University of Jyvaskyla, Finland — We have observed that submicron sized Al–AlOₓ–Al tunnel junctions can be stabilized completely by annealing them in vacuum at temperatures between 350 °C and 450 °C. In addition, low temperature characterization of the samples after the annealing show a marked improvement of the tunneling characteristics, by disappearance of unwanted resonances in the current. Charging energy, tunneling resistance, barrier thickness and height all increase after the treatment. The superconducting gap is not affected, but supercurrent is reduced in accordance with the increase of the tunneling resistance. A useful application of the annealing is in increasing the sensitivity of Josephson junction threshold current detectors, currently used for example in superconducting quantum bit readouts. It is also expected that all other barrier dependent characteristics will also improve (e.g. critical current noise).

11:27AM P43.00002 Gating a two dimensional electron gas in silicon using a metallic single electron transistor. LUYAN SUN, Laboratory for Physical Science, University of Maryland, K.R. BROWN, National Institute of Standards and Technology, Boulder, Co, B.E. KANE, Laboratory for Physical Sciences, University of Maryland — A wealth of physical phenomena has been observed in two dimensional electron systems such as the silicon metal-oxide-semiconductor field effect transistor (MOSFET). Due to impurities and interface states, a silicon /Al SET as the top gate of a conventional MOSFET. The SET is fabricated with standard electron-beam lithography and double-angle thermal evaporation. A thermally grown SiOₓ barrier layer about 20 nm thick isolates the SET from the lightly p-doped MOSFET channel beneath. The drain and source of the MOSFET are heavily n-doped and conduct at cryogenic temperatures. A nearby surface metal gate is used to modulate the width of the channel right beneath the SET island. Near the pinch off regime we expect to see a correlation between fluctuations in the current during the SET and fluctuations in the current of the MOSFET channel. We will present preliminary data from these devices.

Superconducting circuits are a promising system for the implementation of quantum computing. At present two-level system defects in the substrate on which qubits are realized as a significant obstacle to the realization of a superconducting quantum computer. One source of dissipation is through coupling to two-level system defects in the substrate on which qubits are fabricated. To study this effect, loss measurements on LC resonators fabricated on bulk silicon were compared to those fabricated on thin silicon nitride membranes, where much of the substrate material has been removed.

In this talk we will discuss how we define and assess the quality of our shadow evaporated Josephson junctions.

In this talk we will describe efforts to create a quantum information processor using ferroelectrically coupled electron spins in silicon.

The constituent material systems are Ge quantum dots, whose size must be compatible with storage of single electrons, and whose spacing must allow for significant spin exchange to occur. Epitaxial ferroelectric oxides must be capable of rectifying light to allow for optical gating of spin interactions. Progress toward these goals, pursued within the Center for Oxide-Semiconductor Materials for Quantum Computation (COSMQC), will be described. This work is supported by DARPA QuIST through ARO contract number DAAD-19-01-1-0650.

Epitaxial growth of V and MgO films for Josephson junction qubits.

Josephson junctions and the superconducting phase qubits made out of single-crystal Al and single-crystal MgO tunnel barriers, and discuss the effect of barrier crystallinity and electrode/tunnel-barrier interface quality on the performance of the coherent quantum-devices.

The application of average Hamiltonian theory to multiple pulse NMR experiments using finite pulses will be discussed. Through this analysis, we are able to explain an observed pulse phase sensitivity and develop new pulse sequences that exploit and enhance these finite pulse effects. Experiments in both the strong and weak coupling limits will be shown.
11:15AM P44.00001 Universal conductance fluctuations imply excess high frequency noise in mesoscopic gold wires. A. TRIONFI1, S. LEE, D. NATELSON, Rice University Dept. of Physics and Astronomy — In cold, mesoscopic conductors, two-level fluctuators lead to time-dependent conductance fluctuations manifested as 1/f noise that are enhanced by quantum interference up to a universal limit (TDUCF). In Au nanowires, we measure the magnetic field dependence of TDUCF, weak localization (WL), and magnetic field-driven (MF) UCF before and after treatments that alter magnetic scattering and passive surface fluctuators. Our coherence length data resolve a long-standing inconsistency between WL and TDUCF, and may imply that fluctuators produce high frequency noise in excess of 1/f expectations.

1Now with Sandia National Laboratories

11:27AM P44.00002 Low Resistance Interfacing of Single-Crystal Gold Nanowires, BIROL OZTURK, Oklahoma State University, TETSUYA D. MISHIMA, University of Oklahoma, DANIEL R. GRISCHKOWSKY, BRENT N. FLANDERS, Oklahoma State University — We have developed an innovative approach to growing individual, single-crystal gold nanowires between targeted points on lithographic electrodes from simple salt solutions. This approach has allowed us to address a fundamental problem in nano-device-fabrication: the interconnecting of nanowires with external circuitry. That is, we have developed a Labview program which simultaneously controls a function generator and a sourcemeter. This program modulates the growth-inducing voltage to attain low contact resistances between gold nanowires and lithographic electrodes. Four-probe measurements revealed that the contact resistances of the electrode-nanowire-electrode assemblies are consistently less than 25 Ω. To our best knowledge, the sub-25 Ω contact resistances are the smallest that have been attained by any single-step nanowire growth and interfacing approach. Thus, gold nanowires grown with this method are ideal for use as conducting lines in nanoelectronic and nanobiological applications.

11:39AM P44.00003 Long Range Directional Growth of Electrochemical Nanowires, PREM THAPA, BRENT FLANDERS, Oklahoma State University — We report on the directional growth of crystalline metallic nanowires between targeted sites on on-chip circuitry. We observed that 200 nm diameter, needle-shaped wires grow between the electrodes after the deposition of 10 µl aqueous indium acetate solution and application of a 10 MHz alternating voltage. This effect occurs even when the electrodes are separated by as much as 100 µm. Hence, this effect is indicative of a long-range interaction, which is surprising given that this occurs in an electrolytic solution where Debye screening is expected. In this talk, we will discuss the possible origin of this long-range interaction. This capability provides an innovative way to interface multiple nanowires to a single cell membrane, enabling the future study electrophysiological events in live cells.

11:51AM P44.00004 Scanning Tunneling Spectroscopy of Few-Atom Nb Nanoclusters on an Ultrathin Insulating Surface. C.D. RUGGIERO, T. CHOI, J.A. GUPTA, Department of Physics, The Ohio State University — The study of small metallic clusters offers insight into the evolution of electronic structure from atomic orbitals to bulk-like band structure. We report scanning tunneling spectroscopy on small Nb clusters ranging in size from one atom to a few atoms. All data were collected using a low-temperature ultrahigh vacuum scanning tunneling microscope operating at 5K. Insulating islands of CuN (∼5nm x 5nm) were grown on a Cu(100) surface in order to decouple deposited Nb clusters from the metal substrate. Tunneling spectra on a bare CuN island reveal an insulating gap exceeding 4eV despite a thickness of only one monolayer. The dI/dV spectra of few-atom Nb clusters on CuN islands reveal a pronounced peak that may be associated with an atomic resonance. The peak position shifts in energy by as much as 0.5eV as a function of cluster size. http://www.physics.osu.edu/~rgupta

12:03PM P44.00005 Electron transport in magnetite nanoparticles, SUNGBAE LEE, Physics and Astronomy, Rice University, JOHN T. MAYO, VIKKI L. COLVIN, Chemistry, Rice University, DOUGLAS NATELSON, Physics and Astronomy, Rice University — Magnetite (Fe3O4) is an example of a strongly correlated, mixed valence oxide. Electron transport through small numbers of monodisperse magnetite nanocrystals (20nm in diameter) is measured on nanometer-scale three-terminal devices where nanoparticles are decorated on lithographically defined platinum electrodes. The abrupt development of discontinuities on IV curves around 120K and below strongly suggests the particles are going through the Verwey transition. Initial measurements of the full range of IV characteristics and magnetoresistive behaviors of these devices are presented.

12:15PM P44.00006 Strong magnetic scattering from TiO2 adhesion layers1, D. NATELSON, A. TRIONFI2, S. LEE, Department of Physics and Astronomy, Rice University — Electronic phase coherence in normal metals is incredibly sensitive to magnetic scattering. As a result, the weak localization magnetoresistance and time-dependent universal conductance fluctuations are powerful probes of magnetic impurities. We report measurements of these effects in Au and Ag nanowires, comparing samples with and without an underlying 1.5 nm thick Ti adhesion layer. Because of background oxygen, the layer is likely TiOx, with x < 2. Samples with no adhesion layer show no sign of magnetic contamination. Samples with adhesion layers measured immediately after fabrication show clear evidence of strong magnetic scattering. Annealing in air reduces the concentration of scatterers, as does evaporation under conditions that encourage the formation of TiO2. This strongly suggests that the magnetic scattering and its evolution are related to the oxidation state of the Ti, and is consistent with recent reports of ferromagnetism in oxygen-poor TiO2–δ.

1This work was supported by the David and Lucille Packard Foundation and DOE Grant no. DE-FG03-01ER45946/A001
2now at Sandia National Laboratory

12:27PM P44.00007 Quantum Tunneling of Phase Slips in Al Nanowires,1, FABIO ALTOMARE2, Physics Department, Purdue University, W. Lafayette, IN 47906, and Department of Physics, Duke University, Durham, NC 27708 — Superconductivity is a unique phenomenon which manifests itself, most strikingly, as the absence of electrical resistance at very low temperatures. While the resistance in 3-D superconductors — can produce a residual resistance or destroy the superconductivity altogether. In the classical Langer, Ambegaokar, McCumber and Halperin theory, phase slips are caused by thermal excitation over free energy barrier that separates metastable states but Giordano suggested that Macroscopic Quantum Tunneling of phase slips through the barrier (Phys. Rev. Lett. 61, 2137 (1988)) could be significant at very low temperatures where thermally activated phase slips would be exponentially suppressed. However, despite intense experimental effort over the past 20 years, quantum tunneling of phase slips has remained controversial in 1-D superconductors. This talk will discuss the limiting case of 1-D superconductivity in an extremely long (100 µm) and narrow (5 nm–25 atoms) aluminum wire. In applied magnetic field, and at temperatures well below the superconducting transition, we find evidence of macroscopic quantum tunneling at temperatures where the classical theory of thermally activated phase slips would not be able to reproduce the experimental results (Phys. Rev. Lett. 97, 017001 (2006)). Not only are these results valid in linear regime, where most of the experimental data so far has been obtained, but they are consistent and supported by a newly proposed analysis in non-linear regime. These results help ruling out other scenario and establishing that, at temperatures much below Tc, the transport properties of superconducting 1-D nanowires are primarily determined by macroscopic quantum tunneling of phase slips.

1Work supported by NSF No. DMR-0135931 and No. DMR-0401648.
2Present Address: National Institute of Standards and Technology, Boulder, CO 80305
1:03PM P44.00008 Observation of Josephson junction behavior in an individual superconducting NbSe$_2$ nanowire$^1$, ZHIXIAN ZHOU, R. JIN, GYULA ERES, D. MANDRUS, Oak Ridge National Laboratory, Department of Physics, Florida State University, OAK RIDGE, TN 37831, and Materials Science and Technology Division, Oak Ridge National Laboratory, Department of Physics, Florida State University, OAK RIDGE, TN 37831, and Materials Science and Technology Division, Oak Ridge National Laboratory — Resistance and current-voltage characteristics of an individual superconducting NbSe$_2$ nanowire of 75 nm diameter were investigated employing four-probe transport measurements. With the absence of the dissipative motion of vortices, we find that the critical current is limited by a single asymmetric Josephson junction with unequal energy gaps across the junction and that their temperature variation is in excellent agreement with the BCS theory. The difference in the magnitude of the superconducting gap can be attributed to the existence of multiple Fermi surface sheets possessing different electronic structure and electron-phonon interactions. In addition, the temperature dependence of the critical current can be well described by the Ambegaokar-Baratoff relation.

1:15PM P44.00009 Electric Field Effect Modification of Charge Transport in Atomically Thin Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ Nanowires$^2$, ASHER MULLOKANDOV, SOLOMON ENDLICH, JOEL CHUDOW, YUANBO ZHANG, PHILIP KIM, Columbia University, Department of Physics — We investigate the superconducting properties of mesoscopic Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ (BSCCO) crystals of thickness ~2.5-5 unit cells. The crystals are mechanically extracted from the bulk, deposited on a silicon oxide substrate, and 4-probe measurements are conducted with gold contacts. In films that are 3 to 3.5 unit cells thick, the transition from the metallic to the superconducting state is observed at a critical temperature of ~95K, while for 2.5 unit cell crystals the resistance versus temperature curve indicates semiconducting behavior. We also investigate resistance (conductance) variation and critical temperature shifting due to carrier density modulation via an applied gate field at temperatures from 300K to helium temperature. Electric field effect modulation of transport properties in these thin crystallites will be discussed in different temperature ranges.

1:27PM P44.00010 Electron transport studies of superconducting Pb single-electron tunneling transistors, KANG LUO, DONG-HUN CHAE, ZHEN YAO, Department of Physics, The University of Texas at Austin, Austin, TX 78712 — We investigate the electronic transport properties of superconducting Pb single-electron tunneling transistors created by electromigration of Pb nanowires. In the superconducting state, the conductance is suppressed due to the Coulomb blockade effect and the absence of density of states in the superconducting gap. Within the region of suppressed conductance, fine structures are observed which can be attributed to quasiparticle tunneling processes involving singularity matching. These features exhibit strong odd-even parity effect at 2 K and become smeared out at 4.2 K. Our preliminary results of single-molecule transistors using superconducting Pb electrodes will also be presented.

1:39PM P44.00011 Amphoteric Nanocrystalline Quantum Dots, MOHAMMAD ISLAM, American University of Sharjah — The nanocrystalline quantum dot (NQDs) charge states strongly influence their electrical transport properties in photovoltaic and electroluminescent devices, optical gains in NQD lasers, and the stability of the Dots in thin films. We report a unique electrostatic nature of CdSe NQDs, studied by electrophoretic methods. When we submerged a pair of metal electrodes, in a parallel plate capacitor configuration, into a dilute solution of CdSe NQDs in hexane, and applied dc voltage across the pair, thin films of the Dots were deposited on both the positive and the negative electrodes. Extensive characterization including SEM, AFM, FTIR and Raman studies revealed that the films on both the positive and the negative electrodes were identical in every respect, clearly indicating that: 1) a fraction (less than 1%) of the CdSe NQDs in free form in hexane solution are charged and, more importantly, 2) there are equal number of positive and negative CdSe NQDs in the hexane solution. Experiments also show that the number of deposited Dots is at least an order of magnitude higher than the number of initially charged Dots, indicating regeneration. Similar results were seen in maghemite (γ-Fe$_2$O$_3$) NQDs. We used simple thermodynamics to explain such amphoteric nature and the charging/regeneration of NQDs.

1:51PM P44.00012 Fabrication of Variable-Height Nanostructures via Dynamic Stencil Deposition, JEFFREY WASSERMAN, KRISTIN LUCAS, SOO HYUNG LEE, CAITLIN CROWL, ANTHONY ASHTON, JOHN KAYS, Johns Hopkins University — Shadow masks of thin low-stress silicon nitride membranes with nanopore punctures allow for direct deposition of material with features as small as 10nm, without need for resists or other chemical exposure. We have built a device to translate the shadow mask with a nanopore relative to a substrate, allowing controllable nanoscale features to be 'drawn' directly onto the substrate. By modulating the speed of the shadow mask we can vary the height of the nanostructure as it is being deposited. This allows for direct fabrication of nanowires and quantum dots, as well as controllable granular nanostructures and parallel arrays of nanostructures, not feasible using other techniques. We present in this talk our method for implementing nanoscale dynamic stencil deposition, as well as a variety of nanostructures and other components we have fabricated and studied via this deposition technique.

2:03PM P44.00013 Sub-10 nm Device Fabrication in a High-Resolution Transmission Electron Microscope, MICHAEL FISCHBEIN, MARIJA DRNDIC, University of Pennsylvania, Department of Physics and Astronomy — Materials are known to be susceptible to electron-irradiation induced damage during their imaging in a TEM. Though these effects are typically undesirable, we show here that electron-irradiation by the imaging beam of a HRTEM can be used to controllably sculpt metal with single-nanometer precision, thereby enabling device fabrication at a scale that traditional fabrication methods cannot access. We have used this technique to fabricate metal structures with sub-10 nm features on silicon nitride membrane substrates. Examples include arbitrarily curved nanowires, nanometer-wide channels and nanorings. It will be shown that these ultra-small structures can be integrated into large-scale circuitry, without contact resistance. Potential applications of this technique include nanoelectronics, nanofluidics and the study of size effects on superconductivity. This work was supported by ONR Young Investigator Award (N000140410489), NSF Career Grant (DMR-0449553), NSF NSEC Grant (DMR-0425780), and NSF-IGERT (DGE-022166).

Wednesday, March 7, 2007 2:30PM - 5:18PM – Session S9 DMP: Superconductive Tunneling Colorado Convention Center Korbel 1D

2:30PM S9.00001 An asymmetric SQUID for measurement of ultra-small Josephson junctions, D.F. SULLIVAN, Department of Physics, University of Maryland, Laboratory for Physical Sciences, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, Department of Physics, University of Maryland — Ultra-small Josephson junctions offer a variety of potential applications, as well as an opportunity to probe the Josephson effect at the nanoscale. Such junctions, however, are susceptible to fluctuations in the phase difference, γ, across the junction, which leads to a suppression of the critical current I$_{c,0}$. The relevant energies which govern the physics of Josephson junctions are the charging energy E$_C$, the Josephson coupling energy E$_J$, and the thermal energy k$_B$ T. Small junctions have E$_C$/E$_J$ >> 1, while large junctions, with stable critical currents, have E$_C$/E$_J$ << 1. A potential method for stabilizing the phase across a small junction will be presented, which entails shunting it with an additional capacitance C$_1$ and incorporating it in a SQUID loop with another junction having a much larger critical current I$_{c,2}$. The SQUID loop inductance, L, couples γ$_1$ to the stable phase difference γ$_2$ of the large junction. Thus, by properly choosing L and C$_1$, the uncertainty in γ$_1$ should be reduced, allowing a precise measurement of I$_{c,1}$. In addition to the theoretical arguments behind this approach, experimental data incorporating these ideas will be presented. This work was supported by the National Science Foundation.
2:42PM S9.00002 The interplay of the gap, the magnetic resonance, and the van Hove singularity\footnote{This work was supported by the Swiss National Science Foundation}, GIORGIO LEVY, CHRISTOPHE BERTHOD, OYSTEIN FISCHER, DPMC, University of Geneva, Switzerland — The characteristic features of the tunneling spectra in the Bi-based HTS are a $d$-wave like gap structure, strong and often asymmetric coherence peaks, and an asymmetric dip-hump structure at higher energy. Hoogenboom et al. [1] analysed the spectra of the two-layer compound Bi2212 and showed that all of these properties can be understood assuming $d$-wave superconductivity, a band structure as measured by ARPES, and an interaction of the quasiparticles with the magnetic resonant mode. In particular the asymmetric dip-hump results in this model from the interplay of the gap, the mode and the van Hove singularity present in the band structure. Here we analyse new data for the three-layer compound Bi2223. Unlike in Ref. [1], we perform full unconstrained least-square fits in order to determine all parameters of the model directly from the experimental data. This allows us to determine the doping dependence of the gap and of the magnetic resonance energy. [1] B. W. Hoogenboom, C. Berthod, M. Peter, Ø. Fischer, and A. A. Kordyuk, Phys. Rev. B 67, 224502 (2003).

2:54PM S9.00003 Scanning Tunneling Spectroscopy of Bi$_2$Sr$_2$CuO$_{6+x}$ \footnote{Supported by AFOSR, DOE, and KOSEF through CSCMR.}, KAMALESH CHATTERJEE, M.C. BOYER, W.D. WISE, MING YI, MIT, TAKESHI KONDO, Ames laboratory, E.W. HUDSON, MIT — Scanning tunneling microscopy has revealed many interesting spectral features of the high temperature superconductors, including the nature of atomic scale defects like single atom impurities and magnetic vortices and the existence of inhomogeneity. Most of these studies have focused on the bilayer compound Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi-2212). Here we present scanning tunneling microscopy results from its single layer relative, Bi$_2$Sr$_2$CuO$_{6+x}$ (Bi-2211), comparing and contrasting these measurements with previously reported results from Bi-2212.

3:06PM S9.00004 Temperature-Dependent STM Studies of the High Temperature Superconductor BSCCO, MING YI, KAMALESH CHATTERJEE, M.C. BOYER, W.D. WISE, MIT, TAKESHI KONDO, Ames Laboratory, E.W. HUDSON, MIT — Even as the relationship between the superconducting and pseudogap states in high temperature superconductors remains mysterious, scanning tunneling microscopy has revealed a number of similarities and differences between spectroscopy in the two phases. Unfortunately, until now spectra from the same position have not been reported. Here we present results of spectroscopy on identifiable atoms, followed from 4 K to well above the superconducting transition temperature. In particular we will focus on implications for the relationship between the superconducting and pseudogap phases in BSCCO.

3:18PM S9.00005 Point-contact spectroscopy of the pure and Cd-doped heavy-fermion superconductor CeCoIn$_5$, W. K. PARK, L. H. GREENE, Univ. of Illinois at Urbana, J. L. SARRAO, J. D. THOMPSON, Los Alamos National Lab., L. D. PHAM, Univ. of California-Davis, Z. FISK, Univ. of California-Irvine — Point-contact spectroscopy has been performed on pure and Cd-doped CeCoIn$_5$. Conductance spectra of CeCoIn$_5$ along three different orientations exhibit consistent features: i) background asymmetry; ii) Andreev reflection signal over similar energy scales ($\sim$1 meV) and of similarly reduced magnitudes (10 - 13%) at zero-bias.\footnote{Supported by NSF-DMR-0503360 at UCD & UCI, and performed at LANL under auspices of the U.S. DoE, office of Science.} Comparison with the extended Blonder-Tinkham-Klapwijk model calculations indicate the first spectroscopic evidence for $d_{x^2-y^2}$ symmetry of the superconducting order parameter.\footnote{Supported by AFOSR, DOE, and KOSEF through CSCMR.} A two-fluid model\footnote{Supported by AFOSR, DOE, and KOSEF through CSCMR.} will be discussed to explain the asymmetry and the reduced Andreev reflection. Cd-doped (10%) CeCoIn$_5$ exhibits intriguing conductance behaviors as a function of temperature and magnetic field, undergoing antiferromagnetic and superconducting transitions: a broad zero-bias peak below $T_X$ and two competing conductance channels below $T_N$.\footnote{Supported by AFOSR, DOE, and KOSEF through CSCMR.} I.W.K. Park et al., PRB 72, 052509 (2005); cond-mat/0507353; cond-mat/0606535. 2.W.K. Park and L.H. Greene, PRL 96, 259702 (2006). 3. S. Nakatsuji, D. Pines and Z. Fisk, PRL 92, 016401 (2004). Work supported by the U.S. DoE DEFG02-91ER45439 through the FSMRL and the CMM at UIUC, by NSF-DMR-0503360 at UCD & UCI, and performed at LANL under auspices of the U.S. DoE, office of Science.

3:30PM S9.00006 Superconducting gap anisotropy in LuNi$_2$B$_2$C by point-contact spectroscopy\footnote{Supported by the U.S. DoE Award No. DEFG02-91ER45439 through the Frederick Seitz Materials Research Laboratory and the Center for Microanalysis of Materials at UIUC.}, XIN LU, WAN KYU PARK, LAURA H. GREENE, University of Illinois at Urbana-Champaign, JUNG-DAE KIM, SUMMOG YEO, SUNG-IK LEE, Pohang University of Science and Technology, Korea — The superconducting gap anisotropy in non-magnetic members of the intermetallic borocarbide family still remains controversial. Several scenarios have been proposed including the s+g pairing symmetry and multi-band/multi-gap superconductivity. In order to address this issue, especially the puzzle concerning the gap structure of point nodes in the $ab$- and $c$-directions, we applied the point-contact spectroscopy technique to investigate the superconducting gap structure of single crystals LuNi$_2$B$_2$C ($T_c = 16.5$ K) along three different crystallographic orientations. $ab$-plane surfaces are prepared by etching and polishing crystals and their orientations are confirmed by X-ray diffraction. Our preliminary conductance data, analyzed by the one-band Blonder-Tinkham-Klapwijk model, show anisotropic gap values, $\sim$1.6 meV and $\sim$2.6 meV, along (001) and (110) directions, respectively. We will discuss the possible origin for the gap anisotropy.

3:42PM S9.00007 What is local about the Local Density Of States?\footnote{Supported by AFOSR, DOE, and KOSEF through CSCMR.}, REZA JAMEI, JOHN ROBERTSON, EUN-AH KIM, ALAN FANG, AHARON KAPITULNIK, STEVEN KIVELSON, Stanford University — While the influence of impurities on the local density of states (LDOS) in a metal is notoriously non-local due to interference effects, low order moments of the LDOS in general can be shown to depend only on the local structure of the Hamiltonian. Specifically, we show that an analysis of the spatial variations of these moments permits one to “work backwards” from scanning tunneling microscopy (STM) data to infer the local structure of the underlying effective Hamiltonian. Applying this analysis to STM data from the high temperature superconductor, BSCCO, we find that the variations of the electro-chemical potential are remarkably small (i.e., the disorder is, in a sense, weak) but that there are large variations in the local magnitude of the $d$-wave gap parameter.

3:54PM S9.00008 Tunneling DOS of Superconductor / Strong Ferromagnet Bilayers\footnote{Supported by AFOSR, DOE, and KOSEF through CSCMR.}, PAUL SANGIORGIO, MALCOLM BEASLEY, Stanford University, SERGE REYMOND, Université de Lausanne, JUN HYUNG KWON, TESU KIM, KOOKRIN CHAR, Seoul National University — We report tunneling density of states (DOS) studies of superconductor (Nb) / strong ferromagnet (CoFe, Ni) bilayers along with quantitative comparisons with calculations made with the Usadel equation. Since both CoFe and Ni are quite strong ferromagnets, we expect theoretically that the DOS we observe as a function of ferromagnet thickness, $d_F$, should be similar. Instead, we find that the Nb/CoFe superconducting DOS exhibits a scaling behavior with a characteristic length of 0.4 nm, whereas the Nb/Ni superconducting DOS does not scale. Further, the Nb/Ni bilayers have a “double peak” DOS for $d_F = 1.5 - 3.0$ nm and for $d_F = 3.5 - 4.0$ nm, we report the first observation of an “inverted” DOS in a strongly ferromagnetic material. Various modifications to the basic Usadel equation will be compared to the experimental data.
4:06PM S9.00009 Node-like excitations in superconducting PbMo$_6$S$_8$ probed by scanning tunneling spectroscopy . GILLES SANTI, DPMC/MaNEP, University of Geneva, Switzerland, C´EDRIC DUBOIS, Dept of Materials Science and Eng., M.I.T., U.S.A., ALEXANDER PETROVIC, ØYSTEIN FISCHER, DPMC/MaNEP, University of Geneva, Switzerland — We present the first scanning tunneling spectroscopy study on the Chevrel phase PbMo$_6$S$_8$, an extreme type II superconductor with a coherence length only slightly larger than in high-β cuprates. Tunneling spectra measured on atomically flat terraces are spatially homogeneous and show well-defined coherence peaks. The low-energy spectral weight, the zero bias conductance and the temperature dependence of the gap are incompatible with a conventional isotropic $s$-wave interpretation, revealing the presence of low-energy excitations in the superconducting state. We show that our data are consistent with the presence of nodes in the superconducting gap.

4:18PM S9.00010 Superconducting and vortex properties of the β-pyrochlore KO$_2$O$_6$ probed by scanning tunneling spectroscopy . C´EDRIC DUBOIS, Dept of Materials Science and Eng., M.I.T., U.S.A., GILLES SANTI, ØYSTEIN FISCHER, DPMC/MaNEP, University of Geneva, Switzerland — The pyrochlore superconductor KO$_2$O$_6$ was studied by scanning tunneling spectroscopy in both the Meissner and vortex states. In view of the controversy concerning the gap symmetry in this material, several symmetry scenarios were tested against our measured spectra. We find that a very anisotropic (40%) s-like gap accounts best for the measured data. This could be interpreted as the signature of a singlet-triplet mixed state allowed by the absence of inversion symmetry in this compound. Vortices were observed for both magnetic fields considered (2 and 6 T) and were arranged in a hexagonal lattice. From the decay of the zero bias conductance away from the vortex cores, we obtain coherence lengths around 3–4 nm, in line with previous estimates based on $H_c2$.

4:30PM S9.00011 Doping-dependent effect of competing orders (CO) on low-energy quasiparticle (QP) excitations in cuprate superconductivity (SC) sup1, ANDREW BEYER, CHING-TZU CHEN, NAI-CHANG YEH, Physics Dept., Caltech, Pasadena, CA — There is general consensus from experimental and theoretical studies of cuprate superconductors that CO with energies close to the SC gap exist in the cuprates and that at times they can coexist with SC in the ground state. Clarifying the exact role of CO requires both theoretical insight into the microscopic physics and sensitive experimental tools to determine the QP properties. We present an experimental and theoretical investigation of the low-energy QP excitations from coexisting CO and SC in hole-type Bi$_2$Sr$_2$CaCu$_2$O$_8$ and YBa$_2$Cu$_3$O$_6$ and in electron-type La$_2$Sr$_1$CuO$_4$. Our studies involve numerical simulations using a microscopic model of coexisting SC/CO and realistic bandstructures to fit experimental QP tunneling spectra to extract doping dependent CO and SC parameters. We suggest that the low-energy pseudogap is associated with CO being either charge-density waves or disorder-minded spin-density waves but not d-density waves.

1This work is supported by NSF Grant DMR-0405088.

4:42PM S9.00012 The duality of the density orderings in the high temperature superconductor , KANGJUN SEO, JIANGPING HU, Purdue University, HANDONG CHEN, UIUC — We study a d-wave superconductor with possible orders in both the particle-particle and the particle-hole channels using the Bogoliubov-deGennes technique. In the superconducting phase, a duality exists in the particle-particle and particle-hole ordering channels. A small pair density localization generates the d-wave checkerboard density order(DWCB) in the particle-hole channel and the extended s-wave density order(PD$2$) in the particle-particle channel. The mixed state of DSC with DWCB and PDW with $4\times4$ periodicity can explain the checkerboard modulation observed in FT-STS from STM as well as the characteristic features such as non-dispersive Fermi arc in the pseudogap state.

4:54PM S9.00013 Coulomb Interaction-induced Checkerboard Patterns in Disordered Cuprates , DEGANG ZHANG, Texas Center for Superconductivity and Department of Physics, University of Houston, TX 77204 — We study the effect of the Coulomb interaction on the local density of states (LDOS) and its Fourier component in disordered cuprates. It is shown that the Coulomb interaction suppresses strongly the maximum value of the LDOS induced by the dopant impurity at each energy and expands significantly the Friedel oscillation in real space. The existence of the Coulomb interaction with a moderate strength yields an energy-dependent checkerboard LDOS modulation around the impurity, which is very different from that produced by pure quasiparticle interaction. The orientation and transformation of the checkerboard pattern with energy and the relations among the modulation vectors, dopings and the bias voltages agree qualitatively with the recent STM experiments.

5:06PM S9.00014 Atomic Scale Imaging of Quasiparticle Lifetimes in Bi$_2$Sr$_2$CaCu$_2$O$_8$+δ1, J.W. ALLDREDGE, JINHO LEE, Cornell University, K. MCELROY, University of Colorado at Boulder, K. FUJITA, University of Tokyo, M. WANG, J.A. SLEZAK, Cornell University, H. EISAKI, AIST -Tskuba, S. UCHIDA, J.C. DAVIS, Cornell University — Using a d-wave superconductor model with the addition of a $\Gamma_1 + \Gamma_2$Energy term we are able to relate the observed quasiparticle spectrum to two $\Gamma$ parameters which give us the quasiparticle lifetime on the atomic scale. The quasiparticle lifetime is related to classic impurity atoms (zinc) as well as local suppression of the superconductivity at low dopings. The quasiparticle lifetime is shown to change both in spatial distribution and in value as a function of doping. We compare our measured lifetimes to ARPES data and to residual conductance measurements.

1CCMR, CTC

Wednesday, March 7, 2007 2:30PM - 4:54PM — Session S10 DMP: Heavy Fermion Effects in Pu, Ce, and U Colorado Convention Center Korbel 1E

2:30PM S10.00001 Theory of magnetism in Pu at high magnetic fields , PER SODERLIND, Lawrence Livermore National Laboratory — Density-functional theory (DFT), in conjunction with the fixed-spin-moment (FSM) method, spin-orbit coupling (SO), and orbital polarization (OP), is shown to provide an apparent accurate picture of δ-Pu, while opening the possibility of a zero net magnetic moment due to complete spin- and orbital-moment cancellation. Calculated total energies, photoemission spectra, and magnetic form factors appear consistent with available experimental data. Calculations including SO, OP and the Zeeman term in the Hamiltonian, address Pu in high magnetic fields ~ 100 T. The Pu phase stability, as a function of applied field, is also investigated. This work was performed under the auspices of the US DOE by the UC LLNL under contract no. W-7405-Eng-48.
2:42PM S10.00002 Strongly correlated state in $\delta$-Pu and Am1 A. SHICK, Institute of Physics AS CR, Prague, J. KOLOREC, North Carolina State University, Raleigh, L. HAVELA, Charles University, Prague, V. DRCHAL, Institute of Physics AS CR, Prague — We investigate the electron-electron correlation effects in the vicinity of the localization threshold of the 5f series, which is crossed between Pu and Am. The ground state electronic and magnetic properties are calculated making use of static around-mean-field LDA+U approximation. We obtain non-magnetic $\delta$-Pu with 5f occupation $n_f = 5.4$, and non-magnetic $\Delta$-Am with $n_f = 6.0$. The equilibrium volumes and bulk moduli are obtained in a good agreement with experiment. For Pu-Am alloys, neither tendency to a 5f localization nor formation of Pu local magnetic moments was found despite a lattice expansion caused by the Am atoms. The excitation spectra of $\delta$-Pu and $\Delta$-Am are calculated on the basis of the Dynamical Mean-Field theory (DMFT). Starting from LDA+U ground state we investigate multiplet transitions using the Hubbard I approximation [1], which gives a good agreement with experimental photoelectron spectra of $\delta$-Pu, Am, and their selected compounds. The spectral density at Fermi level explains the high $\gamma$-coefficient of the electronic specific heat found experimentally in $\delta$-Pu. The calculations show that atomic-like excitations can be observed in a solid-state environment even if the 5f states are not fully localized as in $\delta$-Pu. [1] A. Shick, J. Kolorec, L. Havela et al., arXiv: cond-mat/0610794 (2006).

2:54PM S10.00003 Dynamical Mean Field Treatment of the Valence Transition in Yb, ERIK YLIVISAKER, UC Davis, ANDREW McMahan, LLNL, WARREN PICKETT, UC Davis — At ambient pressure, Yb metal is a divalent rare-earth with configuration $f^{14}d^1$, where $\nu$ represents the valence $(s, p, d)$ occupation. When pressure is applied it undergoes a gradual transition to a trivalent configuration ($f^{13}d^{14}$), completing by 31 GPa. We investigate this valence transition using the all-electron DMFT(HI) method (which includes 6s, 6p, 5d and 4f in the basis) with the Hubbard I atomic solver. Experimental evidence suggests that this transition involves a linear combination of these two many-body states ($\alpha f^{13}+\beta f^{14}$) with $\alpha$ increasing as pressure is applied. We present evidence that DMFT can appropriately model this type of wavefunction, and that this is necessary to capture the gradual nature of the valence transition in Yb. The DMFT(HI) results are sensitive to the parameter chosen for the $\alpha f^{13}$-$\beta f^{14}$ dependence; however, a good description of the valence transition can be achieved with reasonable adjustments in this function. We also compare and contrast DMFT results with LDA+U, which seems to have fundamental difficulties in modeling this transition. The equation of state provided by the DMFT(HI) method is significantly more accurate than the LDA or LDA+U methods give. More rigorous DMFT (QMC) calculations are currently underway to establish what the accuracy of the HI approximation is.

3:06PM S10.00004 From $\delta$-Pu to PuCoGa$_5$: Kondo effect investigations of strong electronic correlations in Pu1 ERIC D. BAUER, Los Alamos National Laboratory, J. N. MITCHELL, D. S. SCHWARTZ, J. D. THOMPSON, J. L. SARRAO — Within the actinide series, plutonium is located at the itinerant/localized boundary between the strongly hybridized 5f states of U and localized 5f states of Am. The hybridization is intimately connected with the range of interesting behavior found in elemental Pu such as six allotropic phases, the largest effective mass enhancement of any element, and a liquid phase whose density is less than its solid phase, much like ordinary water. Despite decades of research, the strongly correlated electronic state of Pu is still not understood. The exciting discovery of superconductivity in PuCoGa$_5$ with $T_c = 18.5$ K, offers a possibility of understanding strong electronic correlations in Pu. The 5f electrons in PuCoGa$_5$ are neither fully localized nor fully itinerant, similar to the cubic delta phase of Pu. Investigations of the Kondo effect, considered to be the hallmark of strong electronic correlations, in dilute intermetallic systems such as Th$_x$Pu and Lu$_{1-x}$Pu$_x$CoGa$_5$ will yield information about the orbital degeneracy of the Pu 5f electrons, their degree of localization, and a characteristic energy scale of the electronic correlations. Measurements of magnetic susceptibility, electrical resistivity, and specific heat will be presented.

1Work at Los Alamos performed under the auspices of the DOE

3:18PM S10.00005 Ultra-High Magnetic Field Study of Actinide Elements1 CHARLES MIELKE, ROSS MCDONALD, Los Alamos National Laboratory, National High Magnetic Field Laboratory — The magnetic susceptibility and electrical conductivity of elemental plutonium and uranium are predicted to reveal the highly correlated nature of the elements upon application of very intense magnetic fields. A specialized Ultra-High Field generation system has been built and commissioned to study the effects of applied magnetic fields to actinide specimens. Magnetic fields to 150 tesla are routine with maximum field intensity extending to well above 200 tesla. The single turn system is designed to generate fields above 100 tesla while not damaging or dispersing the sample under study. First experimental results will be discussed as well as brief review of the system and techniques.

1This work was supported by the Los Alamos National Laboratory LDRD program, grant number LDRD-DR20070013

3:30PM S10.00006 Volume collapse in Ce alloys under pressure by neutron diffraction1 JAMES L. SMITH, ANNA LLOBET, SERGEI M. STISHOV2, DARRICK WILLIAMS, JASON C. LASHLEY, Los Alamos National Laboratory — Neutron-diffraction measurements under hydrostatic pressure up to 10 kbar were performed on the Ce$_{99.9}$La$_0$Th$_{0.1}$ system to investigate the tricritical point at $x_c = 0.14$. For $x < x_c$, we observe first-order transitions with a pressure derivative of the transition temperature, $dT/dP = 20$ K/kbar. For $x > x_c$, we observe a continuous transition that is second order, which again demonstrates a tri-critical point in the pressure-temperature phase diagram. The results will be presented and discussed.

1Work performed under the auspices of the US DOE.

2also at: Institute for High Pressure Physics of Russian Academy of Sciences, Troitsk

3:42PM S10.00007 Phonon Anomalies in $\alpha$-Uranium1 XIADONG YANG, PETER RISEBOROUGH, Physics Department, Temple University — The temperature dependence of the phonon spectra of $\alpha$-uranium has recently been measured by Manley et al.[1] using inelastic neutron scattering and inelastic x-ray scattering techniques. Although there is little evidence of any anharmonicity, the phonon shows some softening in the optic modes at the zone boundary. In a later publication [2], an extra mode was reported to form at high temperatures, which is incompatible with a structure composed of a monoclinic Bravais lattice with a two-atom basis. We investigate the effect that the f electron-phonon interaction has on the phonon spectrum and its role on the possible formation of a breathing mode of mixed electron and phonon character.


1This work was supported by the award DE-FG01-ER45872 from the US Department of Energy.
Spectral Properties of Elemental Pu Studied by LDA+DMFT, JIAN-XIN ZHU, Los Alamos National Laboratory, A.K. MCMAHAN, Lawrence Livermore National Laboratory, M.D. JONES, University at Buffalo, J.M. WILLS, R.C. ALBERS, Los Alamos National Laboratory — The merger of density functional theory in the local density approximation and the many-body dynamical mean field theory is a powerful theoretical technique for the study of strongly correlated electron materials. We present calculations of spectral properties of the $\delta$-phase plutonium by combining for the first time the sophisticated tight-binding method with a recent implementation of quantum Monte Carlo technique. The tight-binding parameters are determined from the fit to the full-potential linearized augmented plane-wave calculation for the face-centered-cubic crystal structure of the slightly compressed $\delta$-phase plutonium. The computationally more expensive but rigorous quantum Monte Carlo simulation is supplemented by the more efficient but approximate Hubbard-I method. By comparing the calculations without and with spin-orbit interaction included, we discuss our results in the context of several key features observed in the photoemission spectroscopy.

Role of Phonons in Heavy Fermion Volume Collapse within the Periodic Anderson Model, M. A. MAJIDI, J. MORENO, University of North Dakota, B. MORITZ, University of Waterloo, A. MACRIDIN, M. JARRELL, University of Cincinnati, A. K. MCMAHAN, Lawrence Livermore National Laboratory — X-ray and neutron diffraction studies by Jeong et al. indicate the involvement of phonons in the volume collapse of Cerium. Lattice vibrations may also be important in other heavy fermion materials with large volume changes such as Praseodymium. Whether phonons drive the volume change, or the effect has an electronic origin and phonons play a secondary role, is unknown. We address this problem within the Periodic Anderson Model by introducing Holstein phonons coupled with the localized f electrons. We solve this model in three dimensions using the dynamical cluster Quantum Monte Carlo technique to incorporate non-local correlations. In the Kondo regime we calculate the renormalized d-f hybridization with respect to the on-site Coulomb repulsion and the electron-phonon coupling at various temperatures. We also investigate the temperature dependence of the isotropic ionic displacements and compare them with Jeong’s experimental results.

Fermi Surface of the Kondo Lattice Antiferromagnets and Ferromagnets: A Continuum Field Theory Approach, SEIJI YAMAMOTO, QIMIAO SI, Rice University — Studies in the quantum phase transitions of heavy fermion metals have raised the question about the nature of the Fermi surface in a heavy fermion antiferromagnet (AF). Related questions are relevant to their ferromagnetic (FM) counterparts. Here, we study the Kondo lattice model in the limit that the Kondo coupling is small compared to the direct (RKKY) exchange coupling. We map the spin-1/2 Heisenberg Hamiltonian for the local moment component to a quantum nonlinear sigma model. This leads to an effective coupling between a vector boson field and the conduction electrons, which is dominated by the forward-scattering channel. There is also a Berry phase term which can be ignored in the AF case, but must be included in the FM case. We establish that the Fermi surface in the AF case is small [1], and also present the results for the FM case. The implications for the global zero-temperature phase diagram of the FM/AF heavy fermions are discussed. [1] S. J. Yamamoto and Q. Si, cond-mat/0610001

Non-linear Sigma Model of Kondo Lattice in Antiferromagnetic Regime, TZEN ONG, Stanford University, BARBARA JONES, IBM Almaden Research Center — We analyze the antiferromagnetic transition in heavy fermion compounds in two dimensions, which we study using the Kondo-Heisenberg model. The system is assumed to be in the antiferromagnetic regime, with a Heisenberg coupling ($J_{\uparrow\downarrow}$) that is larger than the Kondo coupling ($J_{\downarrow\uparrow}$). The Heisenberg terms are mapped onto a non-linear sigma model, and the fermions are then formally integrated out to obtain an effective theory for the Neel field. We then study the evolution of the Heisenberg and Kondo couplings under renormalization, and calculate the critical exponents at the phase transition. We also find that a mean field calculation of this model gives a pairing state (superconductivity) in part of the $J_{\uparrow\downarrow}$/$J_{\downarrow\uparrow}$ phase space. By symmetry arguments, unless the transition from AFM to SC is first order, this suggests the existence of a new state in between the antiferromagnetic and SC states, and we consider the possibility of a novel new ground state in this regime.

Nonperturbative Scaling of the Disorder Quenched Kondo Effect, STEFAN KETTEMANN, Univ. Hamburg, ANDREY ZHURAVLEV, Univ Hamburg, ISA ZHAREKESHEV, Univ Erlangen, EDUARDO MUCCIOLI, University of Central Florida, SFB668-B2 TEAM, DEPARTMENT OF PHYSICS TEAM — The quenching of the Kondo effect in weakly disordered metals with dilute magnetic impurities is studied by means of the numerical renormalisation group method. Using the one particle basis of a disordered tight binding model on a square lattice of size $L$, we calculate the temperature dependence of the local magnetic susceptibility. We find a finite probability that the magnetic moment remains unscreened at the lowest temperatures. This probability is calculated as function of the exchange coupling $J$, lattice size $L$ and disorder amplitude $W$. These results are compared with analytical and numerical methods, based on the solution of the self consistent 1-loop equation (Nagaoka-Suhl), as well as with the numerical solution of the 2-loop renormalisation group equation. Experimental consequences for disordered metals are studied. In particular, it is shown that the presence of magnetic impurities with small Kondo temperatures enhances the electron’s dephasing rate at low temperatures in comparison to the clean metal case.

Wednesday, March 7, 2007 2:30PM - 5:30PM –
Session S11 DMP: Focus Session: Surfaces of Correlated Electron Systems
Colorado Convention Center Korbel 1F

Are the surfaces of CrO$_2$ metallic? A photoelectron spectroscopy study of epitaxial CrO$_2$(100) and CrO$_2$(110) films, C. A. VENTRICE, JR., Texas State Univ., D. R. BORST, Univ. of New Orleans, H. GEISLER, Texas State Univ., G. X. MIAO, A. GUPTA, Univ. of Alabama — Previous photoelectron spectroscopy studies of CrO$_2$ have found either no density of states or a very low density of states at the Fermi level, suggesting that CrO$_2$ is a semiconductor or a semimetal. This is in contradiction to calculations that predict that CrO$_2$ should be a half-metallic ferromagnet. We present photoelectron spectroscopy measurements of epitaxial CrO$_2$(110)/TiO$_2$(110) and CrO$_2$(100)/TiO$_2$(100) grown using a CrO$_2$ precursor. In addition, measurements of epitaxial Cr$_2$O$_3$(0001)/Pt(111) films grown by thermal evaporation of Cr in an oxygen atmosphere are presented as a reference for reduced Cr$_2$O$_3$ films. The measurements of the CrO$_2$ surfaces show no emission at the Fermi level after sputtering and annealing the surfaces in oxygen, even though our soft core photoemission data and low energy electron diffraction measurements provide evidence that stoichiometric CrO$_2$ is present. The consequence of this is that neither surface of CrO$_2$ is metallic. This behaviour could result from a metal to semiconductor transition at the (110) and (100) surfaces.
2:42PM S11.00002 Surface vs. Bulk Characterizations in Electronic Inhomogeneity of a VO2 thin film. YOUNG JUN CHANG, J.S. YANG, T.W. NOH, ReCOE & FPRD, Department of Physics & Astronomy, Seoul National University, Seoul, Korea. D.-W. KIM, Department of Applied Physics, Hanyang University, Ansan, Kyeonggi 426-791, Korea. J.-S. CHUNG, Department of Physics and CAMDRC, Soongsil University, Seoul 156-743, Korea. E. OH, B. KAHING, School of Physics and Center for Theoretical Physics, Seoul National University, Seoul 151-747, Korea. We have examined the validity of the percolation model for a VO2 thin film using both surface- and bulk-sensitive measurement during the metal-insulator transition (MIT). VO2 is one of the most widely investigated strongly correlated transition metal oxides, and it displays the MIT at around 340K. The metallic surface area fraction obtained by scanning tunneling spectroscopy fails to reproduce conductivity change, whereas the metallic volume fraction extracted by bulk-sensitive techniques confirms the percolative nature of the transport data. This discrepancy suggests that the surface-sensitive techniques require special care in investigating the electronic structures of strongly correlated transition metal oxides which have strong electron-phonon coupling.

2:54PM S11.00003 Mott-Hubbard insulating phases in Sn/Si(111) and Sn/Ge(111) surfaces. GIANNI PROFETA, CNISM, Universita’ degli Studi di L’Aquila, ERIO TOSATTI, International School for Advanced Studies (SISSA), and INFM Democritos and International Centre for Theoretical Physics (ICTP) — The family of surfaces isoelectronic to (1/3) coverage Sn/Si(111), Sn/Ge(111), SiC(0001) includes undistorted (√3x√3) Mott-Hubbard (MH) insulators as well (3x3) periodic distorted 2D metals. Until recently, only SiC(0001) was believed to possess a MH insulating ground state. We conducted a series of LSDA+U calculations where MH states appear disguised as magnetic band insulators – for Sn/Si(111) and for Sn/Ge(111). In Sn/Ge(111) at T = 0, a distorted (3 x 3) metal and a (√3x√3) undistorted MH insulator are found to exist as possible ground states, locally stable and closely competing. This result may explain the recently reported transition of Sn/Ge(111) from a distorted metal to an undistorted MH state at low temperature. [2] In Sn/Si(111) calculations show no stable distorted state, but the ground state turns from a metal to a MH insulator, down to realistically small values of U. This state may just have been discovered experimentally by Modesti’s group.[3]

3:06PM S11.00004 Giant Gap Surface Charge Density Waves in NaMoO3 and KMoO3 surfaces. FENG WANG, S.-K. MO, J. W. ALLEN, U. of Michigan, G.-H. GWEON, UC- Santa Cruz, J. MARCUS, C. SCHLENKER, CNRS, H. HÖCHST, SRC, U. of Wisc. — Quasi-2-dimensional molybdenum bronzes NaMoO3 and KMoO3 have a phase transition into the charge density wave (CDW) state at temperatures (T’s) of 80K and 120K respectively. Our recent angle resolved photoemission spectroscopy (ARPES) data confirm in detail our previous findings [1] of nearly identical electronic structures and well nested Fermi surfaces of these two materials. An important new finding in both NaMoO3 and KMoO3 is the opening of giant energy gaps greater than 0.1 eV at T’s well above the bulk CDW transitions, even as high as 300K. The spectra are very dependent on the sample surface and measurement position, and are strongly time dependent. All the evidence indicates formation of a strongly enhanced surface CDW, in contrast to the interpretation of a recent publication [2] relating these large ARPES gaps to the bulk CDW. We will discuss possible scenarios, e. g. [3], for such surface effects and the implications for measuring the spectral manifestations of the true bulk CDW’s. [1] G.-H. Gweon et al., Phys. Rev. B 55, 13353 (1997). [2] R. Cortes et al, Phys. Rev. Lett. 96, 126103 (2006) [3] S. Modesti, L. Petaccia, G. Ceballos and G. Vobornik, to be published.

3:18PM S11.00005 Strong electron correlation on the Fe3O4(0 0 1) surfaces. HENRY PINTO, Laboratory of Physics, Helsinki University of Technology. P.O. Box 1100, FIN-02015 TKK, Finland. SIMON D. ELLIOTT, Tyndall National Institute, Lee Maltings, Cork, Ireland, ADAM FOSTER, R. M. NIEMINEN, Laboratory of Physics, Helsinki University of Technology. P.O. Box 1100, FIN-02015 TKK, Finland — Magnetite Fe3O4 is a fascinating material that still is not well understood and presents challenges for the state-of-the-art computational methods. This transition metal oxide undergoes a first-order metal-insulator transition at TMI = 120 K. The ferrimagnetic properties of Fe3O4 makes it a promising material for spintronic applications. We use a plane wave density functional theory in the generalized gradient approximation adding a Hubbard-U parameter to describe properly the strongly correlated Fe-3d electrons. Based on previous results we compute the surface structure, magnetic properties and electronic structure of several Fe3O4(0 0 1) surfaces with (√3x√3)R30° reconstruction. The simulated scanning tunneling microscopy images of these surfaces are compared and discussed in the light of available experimental data. Finally, we analyze the possible existence of charge ordering on the Fe3O4(0 0 1) surface and the effect on the surface electronic structure with changing the value of the Hubbard-U parameter on the supercell Fe sites.

3:30PM S11.00006 Electronic structure of the (001) surface of half-metallic manganites. MIGUEL PRUNEDA, UC Berkeley, VALERIA FERRARI, CNEA Argentina, PETER B LITTLEWOOD, EMILIO ARTACHO, University of Cambridge — A good understanding of the physical properties of surfaces and interfaces of in colossal magneto-resistant hole-doped manganese oxides is highly desirable for future applications of these promising materials in magnetoresistive devices for spintronics. We present results for a fully relaxed (001) surface in the optimally doped half-metallic manganites La0.7Sr0.3MnO3 in its distorted orthorhombic phase, based on density functional calculations with explicit doping. The crystal termination gives rise to a splitting in the degenerate t2g and e2g levels, and a surface state with d4z2 and dx2-y2 character develops. The calculations for the relaxed structure show that the tilting of MnO6 octahedra is reduced near the surface, and there is a layer buckling, with a Mn off-centering in the top octahedral layer similar to what observed for Ti in bulk BaTiO3, which decreases rapidly inside the material. As a result of this distortions, the surface state shifts to lower energies, although it is still very localized in the first layer. The Mn off-centering favours the occupation of the conduction d4z2 states, which become more localized and affects the magnetic properties at the surface.

3:42PM S11.00007 A FP-LAPW Study of Atomic Chemisorption on the (100) Surface of δ-Pu. RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, University of Texas at Arlington — Fully relativistic full potential density functional calculations have been performed to investigate atomic carbon, nitrogen, and oxygen chemisorption on the (100) surface of δ-Pu using the all-electron augmented plane waves plus local basis code WIEN2K. The surface was modeled by a three-layer periodic slab with two atoms per surface unit cell. The center adsorption site is found to be the most preferred site with chemisorption energies of 7.964 eV, 7.665 eV, and 8.335 eV for the C, N, and O adatoms, respectively. The corresponding optimized distances of the adatoms from the surface are found to be 0.26 Å, 0.35 Å, and 0.48 Å. The work functions and the net magnet moment increases respectively increased and decreased in all cases compared with the bare δ-Pu (100) surface. Analysis of partial charges inside the atomic spheres, charge density distributions, and the local density of states have been performed to investigate the nature of the interaction between the surface Pu atoms and the adatoms.

3This work is supported by the U. S. Department of Energy and the Welch Foundation.
We report on temperature dependent STM/S measurements of Laser ablated epitaxial thin films (\( \approx 400\)nm thick) of \( La_{0.35}Pr_{0.275}Ca_{0.375}MnO_3 \) (LPCMO) on \( NdGaO_3 \) (NGO) substrate. Four-probe resistivity measurement on this film shows a sharp transition near 145K (\( T_{MI} \)) and a significant hysteresis with temperature between 90K and 160K. The topographic STM images show a clean terraced surface at all temperatures (77-350K) with mono-atomic steps and terrace width of 300-400nm. Some inhomogeneities are observed in the conductance images on a length scale of \( \approx 20nm \) and more apparent near the terrace steps. Although spatial variations in spectra are seen at all temperatures but with some common features that evolve with temperature. The spectra become gap-like below 210K (i.e. \( T_{CO} \)) and with cooling this charge-ordering (CO) gap becomes more pronounced with a magnitude of 0.4-0.5eV. This shows an increase in the strength of the CO order parameter and makes us believe that with cooling the CO fraction in the phase-separation scenario is not decreasing with temperature. In this case the large resistivity change at \( T_{MI} \) may have to invoke a third phase (other than metallic and CO phases) that becomes metallic with cooling rather than CO fraction melting into metallic phase.

---

3:54PM S11.00008 Scanning tunneling spectroscopy study of charge ordering, stripes and phase separation in manganese perovskite oxides. 

**CHRISTOPH RENNER**, London Centre for Nanotechnology, University College London — Colossal magnetoresistance (CMR) in perovskite-based transition metal oxides keeps challenging our understanding. Constant progress in scanning tunneling microscopy investigations is enabling increasingly detailed experimental insight into the different electronic and structural phases nucleating in these complex materials. I shall review the latest findings emerging from experiments on perovskite- and bilayer-manganese [1], which in particular, reveal the importance of lattice degrees of freedom (polarons) and their contribution to the macroscopic transport properties. I shall also discuss the observation of an unexpected hexagonal phase, glimpses of a stripe phase and, finally, address the question of phase separation in these systems.


---

4:03PM S11.00009 Scanning Tunneling Spectroscopy Investigation of \( \text{La}_{2-x-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7 \) (\( x = 0.32, 0.4 \)) at Low Temperatures 

JUNWEI HUANG, JEEHOON KIM, ALEX DE LOZANNE, Department of Physics, University of Texas, J.-S. ZHOU, J. B. GOODENOUGH, Texas Materials Institute, University of Texas — We have investigated the surface electronic properties of the ferromagnetic Ruddlesden-Popper compounds \( \text{La}_{2-x-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7 \) (\( x = 0.32, 0.4 \)) with our home-made ultra-high vacuum (UHV) and low-temperature scanning tunneling microscope at 20K and 80K. We found that the atomically flat surfaces of both compounds show nano-sized features that may be related to the formation of \( \text{Mn}(4+)\)-rich and \( \text{Mn}(3+)\)-rich clusters. The tunneling spectra on these clusters reveal that the local density of states (LDOS) of the \( \text{Mn}(4+)\)-rich clusters is quite different from those of the \( \text{Mn}(3+)\)-rich clusters. We also observed a gap that is temperature dependent and spatially inhomogeneous.

---

4:42PM S11.00010 Spectroscopic Imaging Scanning Tunneling Microscopy Studies of Ruthenates 

M. WANG, JINHO LEE, A. SCHMIDT, Y. KOHSAKA, LASSP, Physics Department, Cornell University, U.S.A., S.A. GRIGERA, School of Physics and Astronomy, University of St. Andrews, U.K., J.C. DAVIS, LASSP, Physics Department, Cornell University, U.S.A. — We report atomic resolution spectroscopic imaging studies of Ruthenates, including \( \text{Sr}_{3}\text{Ru}_2\text{O}_7 \) and \( \text{Ca}_{3}\text{Ru}_2\text{O}_7 \). We will discuss the comparison between ARPES and STM studies of these materials.

---

5:06PM S11.00012 Evidence of Coulomb blockade behavior in finite, one-dimensional quantum well 

VINCENT MEUNIER, MINGHU PAN, ORNL, Oak Ridge, TN, FREDERIC MOREAU, FUNDP, Namur, Belgium, KENNETH PARK, Baylor University, Texas, WARD PLUMMER, ORNL, Oak Ridge, TN and UT, Knoxville, TN — We report on a new type of “quantum box” that is grown on an insulating \( \text{TiO}_2(110) \) surface and is effectively closed by the presence of two charged structures at both ends. The static end charges are responsible for a long-range potential that governs the behavior of the electrons inside the box. As expected from a system with quantum confinement, we observe oscillatory features that can be attributed to standing waves inside the system. The spatial distribution of the charge density fits remarkably well with the solution of the Schrodinger equation, provided that correlation effects are included. However, the astounding result is that they are all observed at room temperature and furthermore unchanged within the range of STM tip potential (about 0.5 V). Because the substrate is insulating and the electrons are well confined inside the structure, we can use the capacitor approach to evaluate the corresponding charging energy. Our theoretical analysis indicates that the energy needed to put an extra electron into the confining structure of \( \approx 14\text{nm} \) amounts to about 1.14-1.30 eV in agreement with a simple classical picture of capacitor charging.

---

5:18PM S11.00013 Surface segregation in \( \text{La}_{2-x-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7 \) (001) 

V.B. NASCIMENTO, R.G. MOORE, H. LIU, The Univ of Tennessee, Knoxville, M.H. PAN, E.W. PLUMMER, Oak Ridge National Lab, Oak Ridge, TN 37831 and Univ of Tennessee, Knoxville, TN 37996, J. RUNDGREN, Royal Inst of Tech (KTH), SE-106 91 Stockholm, Sweden, D. MAZUR, J.W. FREELAND, J.F. MITCHELL, Argonne National Laboratory, Argonne, IL 60439 — The (001) clean surface of \( \text{La}_{2-x-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7 \) with nominal dopings of \( 0.3 < x < 0.4 \) presents a non-magnetic surface layer tentatively explained by the existence of a surface reconstruction. A surface structural investigation of this system was performed using quantitative Low Energy Electron Diffraction (LEED-IV). Results obtained discard the occurrence of a surface reconstruction. However, a strong Sr segregation is observed in these surfaces leading to an effective doping on the surface of \( x = 0.8 \) as well as a possible anti-ferromagnetic phase (in analogy with bulk). Sr segregation is believed to be induced by the creation of a surface which promotes a shift in the phase diagram.

---

1 Work supported jointly by NSF and DOE (DMS) NSF -DMR-0451163, NSF DMR-0346826, U.S. DOE DE-FG02-04ER46125 and by U.S. DOE under Contract No. DE-AC05-00OR22725 with UT-Battelle

Wednesday, March 7, 2007 2:30PM - 5:30PM –
Session S12 GMAG DMP FIAP: Focus Session: III-Mn-V Ferromagnetic Semiconductors Colorado Convention Center Korbel C3
metallic transport of holes within the impurity band. We observe a peak in magnetoresistance at very small magnetic fields.

LYANDA-GELLER, Purdue University, Z. GE, S. SHEN, X. LIU, M. DOBROWOLSKA, JACEK K. FURDYNA, University of Notre-Dame — We investigate the orientation of spins. Our results are consistent with the valence band transport, but consistent with the metallic transport of holes within the impurity band. We observe a peak in magnetoresistance at very small magnetic fields \( B < 20 \) mT, which is independent of orientation of \( B \) with respect to the ferromagnetic easy axis and to the direction of the electric current. The peak appears below 3.4 K and increases at lower temperatures. We attribute this effect to the anomalous negative magnetoresistance of the Aharonov-Bohm (AB) origin. The shape and magnitude of the peak is consistent with weak localization (WL) in a three dimensional (3D) conductor with vanishing spin-orbit interaction. Holes in the valence band, on the contrary, experience strong spin-orbit interaction, which would suppress weak localization in a ferromagnet. In addition to WL we observe a field-independent increase of resistivity at \( T < 5 \) K, a signature of Altshuler-Aronov (AA) electron-electron interaction effect. Temperature dependent AA contribution to resistivity is almost an order of magnitude bigger than the magnitude of magnetoresistance peak, as it should be in conventional 3D disordered conductors.

3:18PM S12.00003 Conclusive Evidence for Impurity Band Conduction in Metallic Ga\(_{1-x}\)Mn\(_x\)As

K.S. BURCH, MPA-CINT, Los Alamos National Laboratory, D.B. SHREKENHAMER, Department of Physics, University of California, San Diego, E.J. SINGLEY, Department of Physics, California State University, East Bay, J. STEPHENS, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, B.L. SHEU, Department of Physics and Materials Research Institute, The Pennsylvania State University, R.K. KAWAKAMI, Department of Physics, University of California, Riverside, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, N. SAMARTH, P. SCHIFPER, Department of Physics and Materials Research Institute, The Pennsylvania State University, D.N. BASOV, Department of Physics, University of California, San Diego — The electronic structure and carrier dynamics of the dilute magnetic semiconductor Ga\(_{1-x}\)Mn\(_x\)As are studied via optical spectroscopy. We focus on the changes induced by annealing the samples, which is known to result in a large increase in the critical temperature. This study provides conclusive evidence that the Fermi energy \( (E_F) \) lies in a metallic impurity band.

3:30PM S12.00004 Insulating ferromagnetic (Ga,Mn)As with low Mn-doping

B.L. SHEU, Physics Department and Materials Research Institute, Penn State University, R.C. MYERS, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, N. SAMARTH, Physics Department, Materials Research Institute, University of California, Santa Barbara, P. SCHIFFER, Physics Department and Materials Research Institute, Penn State University — We probe the onset of ferromagnetism in (Ga,Mn)As near the vicinity of the metal-insulator transition by studying systematic series of low Mn-doped (< 2.0 atomic %) GaAs epilayers [growth described in R.C. Myers et al. Phys. Rev. B 74, 155203 (2006)]. We have studied the temperature dependent magnetization and electronic transport properties of these insulating samples. We fit the data using the variable-range-hopping conduction model and calculate the hopping energy from the logarithm of the resistivity versus \( T^{-1/2} \) slope fit. Our results indicate that a cutoff in ferromagnetism is strongly correlated with critical values of the electric conductivity and the hopping energy. This work is supported by grants from NSF, ONR and DARPA.

3:42PM S12.00005 Imaging of single magnetic dopants in III-V semiconductor hosts

PAUL KOENRAAD, CEM CELEBI, ANDREI SILOV, ANDREI YAKUNIN, Eindhoven University of Technology, JIAN-MING TANG, MICHAEL FLATTE, University of Iowa, MARIA KAMINSKA, Warsaw University, EINDHOVEN UNIVERSITY OF TECHNOLOGY COLLABORATION, UNIVERSITY OF IOWA COLLABORATION, WARSAW UNIVERSITY COLLABORATION — We present room-temperature cross-sectional scanning tunneling microscopy (STM) topographic measurements of the acceptor state wave function for Mn dopants in InP and compare with measurements for the nonmagnetic dopants Zn and Cd as well as with previous results for Mn in GaAs. [1] We find a strong \( 1s \) orbital in the “bow-tie” shape for the Mn acceptor state wave function in InP, similar to those observed in GaAs, which has a binding energy of \( 210 \) meV (compared to 113 meV for Mn in GaAs). The shape for Mn in InP is more symmetric with respect to the 001 plane than Mn in GaAs, which agrees with a general trend for the magnetic and nonmagnetic acceptor state symmetry as a function of acceptor binding energy. We present a new theoretical model based on the surface strain of GaAs (110) that explains why the 001-plane asymmetry of acceptor states seen in STM measurements is much larger than expected from bulk calculations. [1] A. M. Yakunin, et al., Phys. Rev. Lett. 92, 216804 (2004).

3:54PM S12.00006 Atom-by-Atom substitution of Mn in n-type GaAs and Electron mediated Mn-Mn interaction in GaAs

ANTHONY RICHARDELLA, PEDRAM ROUSHAN, DALE KITCHEN, ALI YAZDANI, Princeton Nanoscale Microscopy Laboratory, Department of Physics, Princeton University — Using a novel atomic scale manipulation technique with a cryogenic scanning tunneling microscope (STM), we have recently demonstrated the ability to incorporate single Mn atoms in n-type GaAs substrates and have used this technique to visualize hole-mediated interaction between Mn acceptors in p-type GaAs. [1] We will report on the extension of these experiments to n-type substrates, for which we have also succeeded in incorporation of single Mn acceptors and probed Mn-induced in-gap states using spatially resolved STM spectroscopy. In contrast to previous work, experiments on n-type substrates allow us to explore spin-spin interaction between Mn mediated by electrons in the valence band. Imaging and spectroscopic mapping show Friedel oscillation in the vicinity of individual Mn dopants. We will report these results and more recent experiments on the role of such oscillation on the interaction between Mn-dopants. [1] D. Kitchen, A. Richarcella, J-M. Tang, M. Flatte, A. Yazdani, Nature 442, 436–439 (2006).

4:06PM S12.00007 Anisotropic spin-spin interactions of Mn-Mn pairs in III-V semiconductors

JIAN-MING TANG, MICHAEL E. FLATTE, University of Iowa — We calculate the energy splitting of acceptor states of Mn pairs in GaAs. [1] The calculated splittings show crystalline anisotropy that is in good agreement with recent scanning tunneling measurements [2]. The splitting is large when the pair axis is along the (110) axis and smaller when along the (100) axis. This anisotropy can be understood from the overlap of two Mn acceptor wavefunctions that have the approximate cubic symmetry [3]. Within a double exchange model, the splitting can be linked to the energy difference between parallel and antiparallel Mn spins. Our results show that the parallel configurations always have the lower energy. This exchange coupling energy follows the same crystalline anisotropy for the splitting because the anisotropy is predominately determined by the lowest hole state. The rotational symmetry of the total spin of Mn pairs is weakly broken by the spin-orbit interaction. [1] J-M. Tang and M. E. Flatté, Phys. Rev. Lett. 92, 047201 (2004) [2] D. Kitchen, et al., Nature 442, 436 (2006) [3] A. M. Yakunin, et al., Phys. Rev. Lett. 95, 256402 (2005).
18:00PM S12.00008 X-ray standing wave imaging of Mn in GaAs. JORG ZEGENHAGEN, TIEN-LIN LEE, ISABELLE JOMARD, ESRF, France, MARTIN BRANDT, WSI Munich, Germany, VLADIMIR SCHOCH, University Ulm, Germany — GaMnAs is a prototype of a dilute magnetic semiconductors with a Curie temperature $T_C$ of up to 170 K at a Mn concentration of 5%. Substituting the Ga, the Mn acts as an acceptor with a local spin moment of 5/2 and ferromagnetic ordering is mediated by the itinerant holes. However, depending on the growth conditions and post-growth treatments, small fractions of the Mn may occupy magnetically inactive interstitial sites, act as a donor, compensating the hole doping, and thus decreasing $T_C$. Determining the site distribution of the Mn is therefore important in order to achieve an optimal $T_C$. We used x-ray standing waves generated by substrate (hkl) Bragg reflections to locate the Mn in the GaAs lattice for three differently treated samples, each with 4% Mn in a 4 nm thick epilayer. For 22 reflections, the amplitude as well as the phase of the (hkl) Fourier component of the Mn distribution were determined by recording the Mn K fluorescence during angular scans of the sample traversing the GaAs(hkl) Bragg peaks. Thus a real-space image of Mn within the GaAs unit cell can be reconstructed via direct Fourier expansion. The majority of the Mn is substituting for Ga, but refinement shows that up to 10% of the Mn occupies As interstitial sites.

30:00PM S12.00009 Near field infrared spectroscopy of the ferromagnetic semiconductor Ga$_{1-x}$Mn$_x$As at the nanoscale. G.O. ANDREEV, University of California at San Diego, M. BREHM, F. KEILMANN, Max-Planck-Institut fur Biochemie, Martinsried, Germany, M.M. QAZILBASH, T. DRISCOLL, University of California at San Diego, K.S. BURCH, Los Alamos National Laboratory, J. STEPHENS, D.D. AWSCHALOM, University of California at Santa Barbara, D.N. BASOV, University of California at San Diego — We report on the nanoscale infrared response of a prototypical ferromagnetic semiconductor Ga$_{1-x}$Mn$_x$As at Mn doping fractions in the range of $x=1.8-7.75 \%$. These studies have been carried out using an apertures less scattering Scanning Near field Infrared Microscope (s-SNIM) with a pseudoheterodyne detection scheme operating at the wavelength near 10 $\mu$m. For samples with doping fractions below 7% we observe a contrast-free near field infrared signal, suggesting a homogenous electronic state on the length scale down to 10-20 nm determined by the spatial resolution of s-SNIM. At doping fractions of 7.66% and 7.74% we find significant contrast in the form of surface clusters ranging in diameter from 15 to 30nm in both topographical and near field images. These clusters occupy approximately 15% of the total image area. We will discuss possible origins of the observed contrast within the framework of the effective polarizability dipolar model of the tip-sample interaction.

4:00PM S12.00010 Interlayer Magnetic Coupling in AlBeGaAs/GaMnAs/GaAs/GaMnAs Heterostructures, as Probed with Polarized Neutron Reflectometry. BRIAN KIRBY, National Institute of Standards and Technology, MIKE FITZSIMMONS, Los Alamos National Laboratory, JULIE BORCHERS, National Institute of Standards and Technology, XINYU LIU, ZHIGUO GE, JACEK FURDYNA, University of Notre Dame — Understanding interlayer exchange coupling between magnetic semiconductor layers could prove important for device applications. We discuss a series of AlBeGaAs/GaMnAs/GaAs/GaMnAs heterostructures, fabricated to be identical except for varying GaAs spacer layer thickness. Via hole doping, the AlBeGaAs layer alters the coercivity (Hc) and Curie temperature (Tc) for an adjacent GaMnAs layer. Therefore, in the absence of interlayer coupling, the GaMnAs layers in our heterostructures will not have equal Hc or Tc. Using polarized neutron reflectometry (PNR), we have measured the depth-dependent magnetizations for this series of samples, as functions of applied field and temperature. Our results show the effects of interlayer spacer thickness and temperature on coupling between GaMnAs layers.

5:00PM S12.00011 The role of Mn acceptors in determining the Zeeman splitting of the band edges in GaMnAs. R. CHAKARVORTY, Y.-Y. ZHOU, Y.-J. CHO, X. LIU, J. K. FURDYNA, M. DOBRWOLSKA, Department of Physics, University of Notre Dame, IN 46556 — It has been widely accepted that ferromagnetism in Ga$_{1-x}$Mn$_x$As is carrier-induced, and much work has been devoted to the mechanism of coupling between the Mn ions. However, considerably less attention has been given to the interaction of Mn ions with electronic bands, and to the Zeeman splitting of the band edges. To address the latter issue, we use magnetic circular dichroism (MCD) to investigate how different Mn acceptor states (neutral A$^0$, positively charged A$^+$) affect the magneto-optical properties of Ga$_{1-x}$Mn$_x$As. Several series of Ga$_{1-x}$Mn$_x$As layers were fabricated for this purpose by low-temperature molecular beam epitaxy, using different Mn concentrations (0.001 ≤ x ≤ 0.01), As$_2$ fluxes, growth temperatures and co-dopings. Our MCD data show that in highly compensated samples (i.e., those rich in A$^+$ centers) the Zeeman splitting of the band edges disappears, thus indicating that the exchange between band carriers and Mn spins takes place entirely via the A$^+$ centers.

5:15PM S12.00012 Ferromagnetism in InMnAsP epitaxial films. NIDHI PARASHAR, PHILIP CHIU, BRUCE WESSELS, Northwestern University — The magnetic properties of epitaxial In$_{1-x}$Mn$_x$As$_{1-y}$P$_y$ deposited by metal-organic vapor phase epitaxy were investigated in order to study matrix effects. Alloy concentrations of 0.01 < x < 0.04 and 0.10 < y < 0.25 were evaluated. Films have excellent crystallinity with x-ray rocking curve width of 0.14 degrees. Films were ferromagnetic over the entire composition range studied. The field cooled and zero field cooled magnetization curves exhibit irreversible behavior. A $T_C$ of 318 K was also measured from the field cooled magnetization temperature dependence. Both the irreversibility and the $T_C$ are indicative of the formation of hexagonal MnAs precipitates. The presence of phosphorus promoted the nucleation of hexagonal MnAs precipitates, presumably as the result of the larger mismatch between the matrix and metastable cubic MnAs clusters, as compared to InMnAs.

5:30PM S12.00013 Magnetic Properties of Ga$_{1-x}$Mn$_x$P-based Quaternary Ferromagnetic Semiconductors. P.R. STONE, M.A. SCARPULLA, I.D. SHARP, E.E. HALLER, O.D. DUBON, University of California-Berkeley; Lawrence Berkeley National Lab, E. ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Lab, J.W. BEEMAN, K.M. YU, Lawrence Berkeley National Lab — Ga$_{1-x}$MnP$_x$ is a ferromagnetic semiconductor in which exchange is mediated by carriers localized in a Mn-derived impurity band [Scarpulla et al., Phys. Rev. Lett. 95 207204 (2005)]. Despite its non-metallic nature even for x≤0.042, Ga$_{1-x}$MnP$_x$ displays many properties that are not significantly different from those of the canonical system Ga$_{1-x}$Mn$_x$As including an approximately linear increase of the Curie temperature ($T_C$) with x and a strong spin polarization of the density of states at the Fermi energy. Here we report the effect of partial anion replacement by either S or As on the magnetic properties of Ga$_{1-x}$MnP$_x$-based thin films. In Ga$_{1-x}$MnP$_x$P$_{2-x}$S$_x$ both $T_C$ and X-ray magnetic circular dichroism decrease monotonically with y due to compensation of ferromagnetism-mediated holes by electrons introduced by S. Addition of sulfur significantly enhances the uniaxial magnetic anisotropy between in-plane <110>-type directions with increasingly harder [110] axes as y increases. Finally, we explore Ga$_{1-x}$Mn$_x$As$_{1-y}$P$_y$ for which it has been predicted [Masek et al. cond-mat/0609158v1] that $T_C$ will increase as y increases, thus providing a route to higher $T_C$ based on the well-studied Ga$_{1-x}$Mn$_x$As system.
2:30PM S13.00001 Superconductivity and Unusual Lattice Dynamics in the β-Pyrochlore Oxides. ZENJI HIROI, ISSP, University of Tokyo. Recently two families of pyrochlore oxide superconductors were found: one is α-pyrochlore oxide C$_8$Rh$_2$O$_{17}$ with $T_c=1.0$ K$^2$ and the other is β-pyrochlore oxides A$_2$O$_{2x}$, where A = Cs, Rb and K, with $T_c=3.3$ K, 6.3 K and 9.6 K, respectively.$^2$ The superconductivity of the former compound is of weak-coupling BCS type, while, in the latter compounds, the superconductivity changes from conventional weak-coupling to extremely strong-coupling from Cs to K. In particular, K$_2$O$_{2x}$ with the highest $T_c$ exhibits various unconventional features, which may be ascribed to anomalous electron-phonon couplings arising from the heavy rattling of the K ions.$^3$ Possibly related to this, a first-order phase transition at $T_p=7.6$ K below $T_c$ has been found only for K$_2$O$_{2x}$.$^1$ We will discuss on what is the ratting and how it affects the surrounding conduction electrons in the β-pyrochlorites.

$^3$ Z. Hiroi, S. Yonezawa, Y. Nagao, and J. Yamara, submitted to PRB.

3:06PM S13.00002 Structural Studies of Technetium and Rhenium Oxides$^1$. EFRAIN E. RODRIGUEZ, Materials Research Laboratory, University of California, Santa Barbara & Manuel Lujan Neutron Scattering Center, Los Alamos National Laboratory; FREDERIC POINEAU, Harry Reed Center for Environmental Studies, University of Nevada, Las Vegas; ANNA LLOBET, Manuel Lujan Neutron Scattering Center, Los Alamos National Laboratory; ALFRED P. SATTELBERGER, Argonne National Laboratory; KEN CZERWINSKI, Harry Reid Center for Environmental Studies, University of Nevada, Las Vegas; ANTHONY K. CHEETHAM, Materials Research Laboratory, University of California, Santa Barbara — The oxide chemistry of technetium—99 (t1/2 = 2.12 × 10$^5$ y) has not been investigated to any significant extent and presents an opportunity to explore new structural, electronic and magnetic regimes. The chemistry of rhenium broadly resembles that of technetium, and although ReO$_2$ is a widely studied material with a prototypic structure, it exhibits an unusual thermal expansion evolution that we have studied using neutron powder diffraction. The results of the thermal expansion study will be presented. The structural study of TcO$_2$ and of a new ternary oxide containing technetium and bismuth Bi$_2$T$_x$O$_2$ will be also presented and discussed. Some new reactions of TcO$_2$ and other oxides of heavy elements will be described.

$^1$LANSCE is funded by DOE Office of Basic Energy Sciences.

3:18PM S13.00003 Manifestation of on-site Coulomb and spin-orbit interactions in the ground state electronic structure of Sr$_2$IrO$_4$. HOSUB JIN, JAEJUN YU, Seoul National University — In contrast to the superconducting and metallic ground states in Sr$_2$RuO$_4$ and Sr$_2$RhO$_4$, the ground state of Sr$_2$IrO$_4$ has been reported to be a magnetic insulator. Such an insulating character of Sr$_2$IrO$_4$ is rather surprising and unexpected when the extended nature of Ir 5d state is considered. To investigate the electronic structure of Sr$_2$IrO$_4$, we performed LDA-U calculations taking account of spin-orbit interactions, where both on-site Coulomb interactions and spin-orbit couplings in the description of Ir 5d states are expected to play a significant role. From the results, it is shown that neither the on-site U nor the spin- orbit term only can explain the insulating feature of Sr$_2$IrO$_4$. An interesting interplay between the two competing interactions is found to determine the spin and orbital configuration, leading to a novel insulating ground state. To understand the nature of the ground state, we suggest a minimal model for the t$_{2g}$ manifold based on the tight binding Hamiltonian.

3:30PM S13.00004 Spin-Orbit Coupling Assisted Mott Insulator Sr$_2$IrO$_4$. S. J. MOON, J. S. LEE, M. W. KIM, T. W. NOH, ReCOE & FPRD, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea; H. JIN, B. J. KIM, J. YU, S.-J. OH, CSMCR & FPRD, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea; J.-H. PARK, Pohang Accelerator Laboratory, Postech, Pohang 790-784, Korea, C. KIM. Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea, G. CAO, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA — We have systematically investigated the effect of spin-orbit coupling to the optical conductivity spectra $\chi(\omega)$ of Sr$_2$IrO$_4$. Both Sr$_2$RhO$_4$ and Sr$_2$IrO$_4$ have five d electrons and similar crystal structures. However, Sr$_2$RhO$_4$ and Sr$_2$IrO$_4$ are metallic and insulating, respectively. The insulating ground state of Sr$_2$IrO$_4$ is rather surprising, since it has 5d electrons, which are commonly thought to have extended orbitals. We observed a sharp absorption at about 0.5 eV in $\sigma(\omega)$. This spectral feature cannot be explained in terms of orbital degeneracy and/or density wave. Note that Ir has 5d electrons, so that its spin-orbit coupling should be larger than that of 4d Rh ions. With the aid of the first principles calculation based on the LDA+U scheme, we took into account of the effect of spin-orbit coupling. Our results clearly demonstrate that spin-orbit coupling plays a crucial role to the Mott insulating ground state of Sr$_2$IrO$_4$.

3:42PM S13.00005 Elastic properties of the Mott transition system Ca$_{2-\gamma}$Sr$_{\gamma}$Ru$_2$O$_4$. VEERLE KEPFENS, YANBING LUAN, SRIRAPAN BHATTACHARYA, The University of Tennessee; RONGYING JIN, DAVID MANDRUS, Oak Ridge National Laboratory — Layered perovskite ruthenates have attracted considerable interest since the discovery of superconductivity in Sr$_2$RuO$_4$, which remains the only copper-free superconductor isostuctural to the cuprates. Among the doped varieties of Sr$_2$RuO$_4$, the Ca$_{2-\gamma}$Sr$_{\gamma}$Ru$_2$O$_4$ series is heavily studied, as it connects the Mott insulator Ca$_2$RuO$_3$ with the superconductor Sr$_2$RuO$_4$ and exhibits a variety of physical properties. The current work focuses on the elastic properties of Ca$_{2-\gamma}$Sr$_{\gamma}$Ru$_2$O$_4$. Resonant Ultrasound Spectroscopy (RUS) has been used to measure the resonant frequencies of the samples, which are directly related to the elastic moduli, and results are presented for single crystal samples with $\gamma$ = 0.5, 1.9 and 2.6. The temperature-dependence of the frequencies is found to be quite unusual and reflects the rich phase diagram that sets these materials apart.

$^1$ work supported by NSF-DMR grant 0506292.

3:54PM S13.00006 Strong orbital-dependent $d$-band hybridization and Fermi surface reconstruction in metallic Ca$_{2-\gamma}$Sr$_{\gamma}$Ru$_2$O$_4$. EUNJUNG KO, Department of Physics and IPAP, Yonsei University, Seoul, Korea; B. J. KIM, School of Physics and CSMCR, Seoul National University, Seoul, Korea; C. KIM, HYOUNG Joon CHO, Department of Physics and IPAP, Yonsei University, Seoul, Korea — The layered ruthenate Ca$_{2-\gamma}$Sr$_{\gamma}$Ru$_2$O$_4$ displays diverse ground states ranging from a superconductor ($\gamma$=2) to a Mott insulator ($\gamma$=0), accompanied by structural distortions. We investigate the effects of RuO$_6$ rotation on Ru 4d$^1$ bands structures in the metallic phase (0.5<$\gamma$<2) by first-principles electronic structure calculations. Our study reveals that the symmetry lowering due to RuO$_6$ rotation induces a strong orbital-dependent $t_{2g}$-$e_g$ hybridization. As a result, only the $d_{xy}$ band among three $t_{2g}$ bands is severely affected and thereby the Fermi surface is reconstructed, forming a new electron-like $d_{xy}$ Fermi surface near $\Gamma$ and nested sections near $x$=0.5. These findings should provide a new insight on the electron correlation in the material.

$^1$ This work is supported by the BK21 Project. Computational resource is provided by KISTI under the 7th Strategic Supercomputing Support Program.
4:06PM S13.00007 Surface Structural Phases of Ca$_{2-x}$Sr$_x$RuO$_4$¹

R. G. MOORE, V. B. NASCIMENTO, Univ. of Tennessee, Knoxville, TN 37996. JIANDI ZHANG, University of Tennessee-Knoxville, MIAMI, FL 33199, ISMAIL NILS, R. JIN, J. MANDRUS, E. W. PLUMMER, Oak Ridge National Lab, Oak Ridge, TN 37831 and Univ. of Tennessee, Knoxville, TN 37996 — Surface structural phases of Ca$_{2-x}$Sr$_x$RuO$_4$ (CSRO) are investigated using Low Energy Electron Diffraction (LEED-IV). The surface structure and phases are compared to the bulk in this layered perovskite material. Bulk phases are generated from rotational and tilt distortions of the RuO$_6$ octahedral. While the surface emphasizes the system’s instability against the rotational distortion, the tilt distortion is stabilized. Surface relaxation interferes with the RuO$_6$ tilt resulting in a lower metal-to-insulator transition (MIT) temperature ($x = 0.1$) and a lower tetragonal-to-orthorhombic phase transition temperature ($0.2 < x < 0.5$). In addition, structural transitions accompanying the bulk MIT are nonexistent on the surface for $x = 0.1$ and superstructure reflections are evident for $x = 0.5$ indicating a shift in the quantum phase at the surface.

¹Supported by NSF and DOE (DMS) NSF -DMR-051163, NSF DMR-0346826, U.S. DOE DE-FG02-04ER46125 and by U.S. DOE under Contract No. DE-AC05-00OR22725 with UT-Battelle.

4:18PM S13.00008 Dopant-Induced Nanoscale Electronic Inhomogeneity in Ca$_2$-xSr$_x$RuO$_4$²

JIANDI ZHANG, Florida International University, ROB MOORE, University of Tennessee-Knoxville, SHANCAI WANG, HONG DING, Boston College, RONGYING JIN, DAVID MANDRUS, Oak Ridge National Laboratory, WARD PLUMMER, University of Tennessee-Knoxville — Ca$_{2-x}$Sr$_x$RuO$_4$ single crystals with $0.1 \leq x \leq 2.0$ have been studied systematically using scanning tunneling microscopy (STM) and spectroscopy (STS), low-energy electron diffraction (LEED), and angle resolved photoelectron spectroscopy (ARPES). In contrast to the well-ordered lattice structure, the local density of states (LDOS) at the surface clearly shows a strong doping dependent nanoscale electronic inhomogeneity, regardless of the fact of isovalent substitution. Remarkably, the surface electronic roughness measured by STM and the inverse spectral weight of quasiparticle (QP) states determined by ARPES are found to vary with $x$ in the same manner as the bulk in-plane residual resistivity, following the Nordheim rule. For the first time, the surface measurements—especially those with STM—are shown to be in good agreement with the bulk transport results, all clearly indicating a doping induced electronic disorder in the system.

²Supported by NSF DMR-0346826, DMR-0353108, DMR-0451163, DOE DE-FG02-04ER46125, DOE DMS, and ORAU faculty summer research program. The work at Oak Ridge National Laboratory was supported through DOE under Contract AC05-00OR22725.

4:30PM S13.00009 Antiferromagnetic metallic state: A transport and thermodynamic study of Ca$_{3}$((Ru$_{1-x}$Cr$_x$)$_2$O$_7$)²

V. DURAIRAJ, S. CHIKARA, G. CAO, University of Kentucky, Lexington, KY40506, P. SCHLOTTMANN, Florida State University — Among the variety of exciting physical properties, a signature feature of the bilayered Ca$_3$Ru$_2$O$_7$ is the antiferromagnetic metallic (AFM) state that lies between a Neel temperature, $T_N$=56 K and a Mott-like transition (MIT), $T_{M1}$=48 K. The results of our recent thermodynamic and transport study of single crystal Ca$_3$((Ru$_{1-x}$Cr$_x$)$_2$O$_7$) reveal that the temperature regime of the AFM state is significantly broadened with $x$ increasing in the range of $T_{M1} < T < T_N$. In addition, the magnetic easy axis for magnetization moves gradually away from the a-axis to the b-axis as $x$ increases and at $x=0.20$, the magnetic anisotropy in the basal plane diminishes. This reduced spin polarization along the easy axis is promptly reflected in the less pronounced negative magnetoresistance as $x$ increases. Furthermore, the DC current–voltage characteristics show the S-shaped negative differential resistivity for $x=0.17$. As seen in the pure compound, observed non-ohmic behavior is restricted to the AF nonmetallic region. All results are presented along with comparisons drawn from related systems such as perovskite Ca$_3$Ru$_2$O$_7$/Ag tunnel junctions where highly anisotropic magnetism is induced by Cr substitution. * This work was supported by NSF grants DMR-0240813 and DMR-0552267.

4:42PM S13.00010 Effects of Doping on the Field-dependent Phases of Ca$_3$Ru$_2$O$_7$³

J. F. KARPUS, S. L. COOPER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois Urbana-Champaign, G. CAO, Department of Physics and Astronomy, University of Kentucky — The double-layer ruthenate Ca$_3$Ru$_2$O$_7$ has been shown to possess a rich magnetic-field dependence for fields applied in the a-b plane. In its ground state, Ca$_3$Ru$_2$O$_7$ is an antiferromagnetic insulator, turning metallic above $T_{M1}=48$ K and paramagnetic above $T_N=56$ K. Light doping with Sr ($r=1.18$ Å vs. $r=1.00$ Å for Ca) causes a reduction in the anisotropy field due to the change in lattice parameter along the c-axis, thereby giving us a bandwidth control, while doping with trivalent La ($r=1.03$ Å) not only alters the bandwidth but also adds an extra electron for filling control. Using Raman scattering we map out the orbital, magnetic, and conducting phases by studying the field- and temperature-dependence of the magnetic and vibrational spectra. In this talk we describe the role Sr- and La- doping has on the field dependent phases of (Ca$_3$Sr$_x$L$_{3-x}$)Ru$_2$O$_7$. Work supported by NSF DMR02-44502, NSF DMR-0240813, and DOE DEFG02-91ER45439.

4:54PM S13.00011 Measurement of the Mott insulating gap in Ca$_3$Ru$_2$O$_7$ by tunneling spectroscopy

ANTHONY BAUTISTA, V. DURAIRAJ, S. CHIKARA, G. CAO, K.-W. NG, University of Kentucky — The bilayered Ca$_3$Ru$_2$O$_7$ adopts an orthorhombic structure with the tilt orientation of RuO$_6$ octahedra in the basal plane. It is thus highly anisotropic magnetically and electronically. The extensive d-electron orbitals generate strong coupling between spin-orbit and lattice, resulting in an exotic ground state and leading to interesting properties at low temperatures. For instance, it undergoes a transition from a paramagnetic metallic state to an antiferromagnetic metallic state as the temperature is lowered to 56K, and subsequently another transition, a Mott transition, at a lower temperature of 48K. We have prepared Ca$_3$Ru$_2$O$_7$/Al$_2$O$_3$/Ag tunnel junctions to measure the density of states of Ca$_3$Ru$_2$O$_7$ at low temperatures. The Mott insulating gap is determined to be $-0.076$ eV when it first opens up at 48K, but the gap continues to grow with decreasing temperature. In some junctions, the density of states displays unusual activities in the temperature range of the antiferromagnetic metallic state, between 48K and 56K. Results of this study, in particular the temperature dependence of the gap structure in the density of states will be presented and discussed.

5:06PM S13.00012 Quantum criticality and coexistence of spontaneous ferromagnetism and field-induced metamagnetism in triple-layered Sr$_x$RuO$_{1.5}$¹

SHALINEE CHIKARA, VINOBALAN DURAIRAJ, GANG CAO, JOSEPH W. BRILL, Department of Physics and Astronomy, University of Kentucky, Lexington, KY40506, PEDRO SCHLOTTMANN, Department of Physics, University of Florida State University, Tallahassee, FL - Results of a thermodynamic and transport study of Sr$_x$RuO$_{1.5}$ as a function of temperature and magnetic field are presented. The central results of this work include growing specific heat $C$ with increasing field $B$, divergent magnetic contribution to $C$ at low temperatures, an abrupt jump and a peak in $C/T$ at $B=2.90$ T and $T=7$ T for $B$[ab-plane and $B$[c-axis, respectively, and corresponding changes in the power law of resistivity. All results provide not only strong evidence for metamagnetic quantum criticality but also quantum fluctuations in a spontaneously ferromagnetic state. The novelty of this work lies in the fact that the quantum criticality occurs in a system that shows both intralayer metamagnetism and interlayer spontaneous ferromagnetism, a feature characteristically different from all other relevant systems involving quantum criticality.

¹This work was supported by NSF grants DMR-0240813 and DMR-0552267 and DOE grant DE-FG02-98ER45707.
Evidence of strong disorder in both the ferromagnetic and antiferromagnetic phases of SrRu$_{1-x}$Mn$_x$O$_3$ using the Mössbauer Effect$^1$, MICHAEL DEMARCO, B. GRAVES, G. HARMON, N. MILLER, D. COFFEY, Dept. of Physics, Buffalo State College, NY 14222, B. DABROWSKI, S. KOLESNIK, M. MAXWELL, Dept. of Physics, Northern Illinois University, IL 60115, S. TOORONGIAN, M. HAKA, Nuclear Medicine Department, SUNY Buffalo, NY 14260 — We investigate the magnetism and disorder in powder samples of SrRu$_{1-x}$Mn$_x$O$_3$ and find significant changes in the Mössbauer spectra even at very low values of $x$. At $x = 0.1$, although the width of the spectrum is consistent with a hyperfine field $\sim 32T$, this is similar to that of SrRuO$_3$(33T), a single site fit fails, suggesting that there is a range of RuO$_6$ octahedra distortions. This sensitivity to doping is also seen in the spectrum of CaRu$_{0.8}$Cr$_{0.2}$O$_2$, where there is a $\sim$30T wide distribution of hyperfine fields. At $x = 0.9$ the hyperfine field is due to antiferromagnetic order and is much larger, 90T, than at $x = 0.9$. The charge state of the Ru atom has also changed from +4 to close to +5. Again the spectrum is not that of a single Ru site in spite of the low density of Ru atoms in the sample.

$^1$ The work was supported by the USDOE(DE-FG02-03ER46064) at BSC and by the NSF(DMR-0302617) at NIU.

2:30PM S14.00001 Spin Transfer Switching and Magnetization Dynamics in Py/Cu/Py Nanopillar Spin-Valves with Sidewall Oxide Passivation and Nonuniform Current Injection, OZHAN OZATAY, KEE WEE TAN, PRAVEEN GOWTHAM, PATRICK M. BRAGANCA, ERIC MICHAEL RYAN, GREGORY D. FUCHS, JOHN C. READ, ANDRE K. MKHOYAN, MALCOLM G. THOMAS, KIRAN V. THADANI, JACK C. SANKEY, JOHN SILCOX, DANIEL C. RALPH, ROBERT A. BUHRMAN, Cornell University — The manipulation of magnetization, both to drive precessional dynamics and trigger magnetization reversal in nanomagnets by transferring spin angular momentum from a spin-polarized current, presents opportunities for better scalability in nanoscale magnetic memory devices and microwave oscillators. Some of the major practical concerns include reducing the current level needed to write magnetic bits in an error-free fashion at high operating speeds in memory devices as well as exciting highly coherent dynamic modes for nanoscale microwave oscillator applications. In this work we report on the detrimental effects of the adventitious antiferromagnetic oxides at the perimeter of Py/Cu/Py nanomagnets such as an anomalous increase in magnetic damping at low temperatures and stochastic fluctuations in switching fields. We find that in addition to sidewall oxide passivation, the concentrated spin torque from nonuniform injection also reduces the sidewall effects leading to a more efficient spin transfer switching mechanism as well as microwave dynamics.

2:42PM S14.00002 Current-Induced Magnetization Switching (CIMS) for ‘Ballistic’ and ‘Diffusive’ Transport Through the Non-Magnetic (N) metal in Permalloy/N/Permalloy Nanopillars, NIKOLETA THEODOROPOULO, AMIT SHARMA, MUSTAFA ALHAJ-DARWISH, WILLIAM PRATT JR., JACK BASS, Physics Department, Michigan State University —. Adding 5% Ge to Cu decreases the mean-free-path, $\lambda$, at 4.2K from $\sim 130$ nm to $\sim 3.8$ nm, while still leaving the spin-diffusion length $\gtrsim 40$ nm. Thus, comparing the CIMS switching currents at 4.2K for sputtered Py/N/Py with layer thickness $t_{\text{Cu}} = 10$nm for $N = \text{Cu}$ or Cu(5% Ge), allows testing of the importance of “quasi-ballistic”--($t_{\text{Cu}}/\lambda_{\text{Cu}} \sim 0.08$, versus “quasi-diffusive”--($t_{\text{Cu}}/\lambda_{\text{Cu}} \sim 2.6$), transport, with at most minor correction for spin-flipping in the N-metals. At 4.2K we find a ratio of switching currents, $\Delta I_{\text{CuGe}}/\Delta I_{\text{Cu}} = 1.3 \pm 0.2$, where $\Delta I_{\text{Cu}}$ is the sum of the magnitudes of the critical current for switching from parallel to anti-parallel magnetic order and vice-versa. We will compare this ratio with values calculated using different models.

2:54PM S14.00003 Temperature dependence of current induced magnetization switching in spin-valves with a ferrimagnetic CoGd free layer, LI GAO$^1$, XIN JIANG, IBM Almaden Research Center, San Jose, CA 95120, JONATHAN SUN, IBM T. J. Watson Research Center, Yorktown Heights, NY 10598, STUART PARKIN, IBM Almaden Research Center, San Jose, CA 95120 — Current induced magnetization switching (CIMS) has stimulated great interest recently due to its potential for applications, such as magnetic random access memories. Here, we report for the first time, a CIMS effect in spin-valves with a ferrimagnetic CoGd free layer. The temperature dependence of the CIMS effect in CoGd-Cu-CoFe spin-valves is explored. At temperatures well above and well below the magnetization compensation temperature ($T_{MC}$) of CoGd, a current flowing from the free layer to the CoFe fixed layer aligns the moments of the two layers parallel, and a current flowing in the opposite direction aligns them antiparallel. However, for intermediate temperatures just above $T_{MC}$, the current-induced alignment of the moments is reversed. We attribute this to the different compensation temperatures of the net magnetization and angular momentum of CoGd.

3:06PM S14.00004 Spin-torque-induced reversal in nanopillars containing perpendicularly magnetized layers, ERIC FULLERTON, Hitachi GST — Devices where at least one of the magnetic elements has the anisotropy normal to the film surface are theoretically predicted to increase the efficiency and/or the speed of spin-torque switching. Devices where both the layers have the magnetization normal to the surface increase the efficiency of reversal while devices that combine perpendicular and in-plane magnetized layers are predicted to increase the speed of switching. In this talk we describe recent experimental demonstrations of current-induced magnetic reversal of magnetic elements with perpendicular anisotropy and high coercive fields. The best results are observed for Co/Ni multilayers, which exhibit higher giant magnetoresistance values and spin-torque efficiencies than Co/Pt multilayers. The sample structures are nanopillars with a Co/Pt/Co/Ni composite reference magnetic element and a Co/Ni free layer that responds to the current. The reference layers were designed to have significantly higher anisotropy and coercive allowing a complete current-field phase diagram of the free layer to be explored. The results are compared to micromagnetic modelling that, depending on the bias current and applied field, details regions of irreversible magnetic switching, coherent and incoherent spin waves, or static non-uniform magnetization states. Whereas only the two uniform magnetization states are available under the action of a magnetic field, we observed current induced Bloch domain walls in pillars as small as 100x50 nm². This domain wall state can be further controlled by current to restore the uniform states. This ability to manipulate high-anisotropy magnetic elements could prove enabling for a range of spintronic applications. This research is done in collaboration with S. Mangin, D. Ravelosona, Y. Lemaho, Y. Henry, J. Katine, M. Carey, and B. Terris.

$^1$Dept of Applied Physics, Stanford Univ, Stanford, CA 94305
3:42PM S14.00005 Ferromagnetic resonance studies of nanopillars with Co/Ni multilayer free layers, WENYU CHEN, J-M. L. BEAUJOUR, G. DE LOUBENS, ANDREW D. KENT, New York University, M. J. ROOKS, N. RUIZ, JONATHAN Z. SUN, IBM T. J. Watson Research Center — Recently it has become possible to study ferromagnetic resonance (FMR) of magnetic layers in nanopillar junctions using the spin-transfer interaction [1,2]. This enables powerful new quantitative studies of the layer magnetic anisotropy and damping in confined structures. Here we report studies of Co/Ni multilayer free layers with variable easy plane anisotropy. Experiments were conducted on [(t nm Co 2t nm Ni)] x 1.2/(t) 10 nm Cu] 12 nm Co] layer structures patterned to ~50 nm lateral dimensions using a nanostencil process, with t=0.1, 0.2, 0.3 and 0.4. Varying the Co thickness (t) enables systematic variation of the Co/Ni easy-plane anisotropy, while the total magnetic moment and thickness of the free layer is kept constant. Field swept FMR measurements were conducted using a microwave signal generator (1 to 20 GHz) with a magnetic field applied perpendicular to the surface of the layers. The resonace field and linewidth were measured as a function of frequency and DC current bias. Magnetic anisotropy constants and damping parameters are determined and compared to those found in FMR studies of extended films of the same layer structure. [1] A. A. Tulapurkar et al., Nature, 438, 339 (2005) [2] J. C. Sankey et al., Phys. Rev. Lett., 96, 227601 (2006)

3:54PM S14.00006 Reducing the critical switching current of magnetic multilayers — an ab-initio approach, PAUL HANEY, U. Texas at Austin, DEREK WALDRON, McGill University, ALVARO NUNEZ, Instituto de Fisica, PUCV, REMBERT DUINE, Utrecht University, HONG GUO, McGill University, ALLAN MACDONALD, U. Texas at Austin — We examine strategies for reducing the critical switching current density of spin valve structures, including the dual spin filter (DSF) design, and the use of depolarizing materials outside of the magnetic layers. We study both ideas from first principles using the non-equilibrium Green’s function formalism and direct microscopic evaluation [1] of spatially resolved spin transfer torque contributions. We compare the spin torques present in simple Co-Cu-Co sandwiches with those in the DSF structure. In addition we study the role of Ru layer in enhancing the spin transfer efficiency, exploring the physical origin of Ruthenium’s apparent usefulness in microscopic detail. [1] Haney et al.: cond-mat/0611534

4:06PM S14.00007 Spin-Motive Force Studies in Spin-Valves, JUN’ICHI IEDA, SADAMICHI MAEKAWA, CREST JST; IMR Tohoku Univ., STEWART BARNES, Physics Dept., Univ. of Miami — A spin-motive force (smf) is the counterpart of an electro-motive force, which couples to spin degrees of freedom of electrons rather than charge ones. Here we discuss how the smf works in the so-called spin-valves. Usually the observed dV/dI or in spin-valves is analyzed in terms of magneto-resistance. However when the magnetization makes a sudden jump, there often appears a large peak in dV/dI, i.e., a voltage jump that is better interpreted in terms of the smf discussed here. In order to see this, we model spin-valves using an equivalent circuit that involves magnetic dissipation represented by the smf as well as electric dissipation through ordinary resistors for both majority and minority currents. There are four possible conduction paths, e.g., the majority electrons tunnel into the majority band, or into the minority band and vice versa. The first path adds an up electron to the free layer and causes a rotation in a certain sense, while the second path adds a down electron and a rotation in the opposite sense. Since the rotations are in opposite senses so is the work done on the free layer and hence the smf. The equivalent circuit with the relevant parameters predicts a stable large angle precession and the voltage signal.

4:18PM S14.00008 Magnetooptanto and spin-torque effects in current perpendicular to the plane spin-valves with Co–Fe–Al magnetic layers, STEFAN MAAT, MATTHEW CAREY, JEFFREY CHILDRESS — The magneto-optic transport of current-perpendicular to the plane giant magneto-resistive spin valves utilizing (Co,Fe)100−x−yAl25 alloys in the reference and free layers is investigated. (Co80Fe20)75Al25 is determined to be the alloy composition that maximizes magneto-resistance. At this composition the magnetization is around 1000 emu/cm3, which is high enough to be used as magnetic material in spin-valves with ultra-thin read gaps for high recording densities. An improvement in magneto-resistance from 1.7% for spin-valves utilizing Co80Fe20 in reference and free layers to 3.3% for spin-valves utilizing (Co80Fe20)75Al25 with the same “magnetic” thickness in both parts of the reference and the free layers were observed. The spin-diffusion length for (Co80Fe20)75Al25 is determined to be approximately 30 Å. Spin-torque measurements show that the spin-torque current density threshold is approximately 107 A/cm2 in CoFeAl spin-valves in comparison to 105 A/cm2 in CoFe spin-valves.

4:30PM S14.00009 Magnetization and resistance noise in spin valves, Joon FOROS, ARNE BRATAAS, Department of Physics, Norwegian University of Science and Technology, GERRIT E. W. BAUER, Kavli Institute of NanoScience, Delft University of Technology, YAROSLAV TSERKOVNYAK, Department of Physics and Astronomy, University of California — Electronic noise hinders the application of spin valves as read heads in magnetic hard drives. We report a theoretical analysis of such noise. Electronic or resistance noise in spin valves is caused by fluctuations in the relative orientation of the magnetic layers via the magnetoresistance-effect. Two sources of thermal magnetization fluctuations can be distinguished: Random fields intrinsic to the bulk ferromagnets, and external spin current fluctuations that affect the magnetizations through the spin-transfer torque. The cross talk between fluctuating magnetizations and the corresponding resistance noise strongly depends on the magnetic configuration. In agreement with experiments by Covington et al. [1] we find that the noise level in the antiparallel configuration can exceed that of the parallel one by an order of magnitude.

1M. Covington et al., unpublished

4:42PM S14.00010 Effect of Bias on Spin-Transfer Torque in Magnetic Tunnel Junctions, IOANNIS THEODONIS, ALAN KALITSOV, NICHOLAS KIOUSSIS, Department of Physics, California State University, Northridge, MAIRBEK CHSHIEV, W. H. BUTLER, MINT Center, University of Alabama — The current-induced magnetic switching in non-collinear magnetic tunnel junctions (MTJ) through the spin-transfer torque (STT) provides the possibility of manipulating nonvolatile MRAM, without applying cumbersome magnetic fields. Using tight-binding calculations and the non-equilibrium Keldysh formalism, we have studied the effect of applied bias on the components of the STT, parallel T¶, and perpendicular, T⊥, to the interface. We show that depending on the exchange splitting, T¶ may exhibit a non-monotonic bias dependence: it may change sign without a sign reversal in current, and in some cases it may even have a quadratic bias dependence. Second, we show that T⊥ is given by the difference in spin currents between the FM and anti-ferromagnetic (AF) configurations. Third, the bias dependence for the spin current for the FM (AF) alignment is shown to have a linear (quadratic) bias dependence, whose origin lies on the symmetric (asymmetric) nature of the barrier. The interplay of the spin currents for the FM and AF configurations can lead to a rich behavior of the T¶ on bias. Finally, we find that, T⊥ (non-equilibrium exchange coupling), is comparable in size with T¶, and has a quadratic bias dependence.

1Department of Physics, National Technical University, Gr-15773, Zografou, Athens, Greece

Wednesday, March 7, 2007 2:30PM - 5:30PM – Session S20 DMP: Focus Session: Nanoscale Ferroelectrics, Switching, and Domains

Colorado Convention Center 105
2:30PM S20.00001 Probing nanoscale ferroelectricity by ultraviolet Raman spectroscopy1. DMITRI TENNE, Boise State University and Pennsylvania State University — Conventional vibrational spectroscopies operating in visible and infrared range fail to measure the phonon spectra of nanoscale ferroelectric structures because of extremely weak signals and the overwhelming substrate contribution. In this talk, application of ultraviolet (UV) Raman spectroscopy for studies of lattice dynamics and ferroelectric phase transitions in nanoscale ferroelectrics will be presented. We demonstrate that UV Raman spectroscopy is an effective technique allowing the observation of phonons and determination of the ferroelectric phase transition temperature (Tc) in nanoscale ferroelectrics, specifically, BaTiO3/SrTiO3 superlattices having the ferroelectric BaTiO3 layers as thin as 1 unit cell and single BaTiO3 layers as thin as 4 nm. BaTiO3/SrTiO3 superlattices and ultrathin BaTiO3 films studied were grown by molecular beam epitaxy on SrTiO3 as well as GdScO3 and DyScO3 substrates. Excellent epitaxial quality and atomically abrupt interfaces are evidenced by X-ray diffraction and high resolution transmission electron microscopy. UV Raman results show that one-unit-cell-thick BaTiO3 layers in BaTiO3/SrTiO3 superlattices are ferroelectric with the Tc as high as 250 K, and induce the polarization in much thicker SrTiO3 layers adjacent to them. The Tc in superlattices was tuned by hundreds of degrees from ∼170 to 650 K by varying the thicknesses of BaTiO3 and SrTiO3 layers. Using scandate substrates enables growth of superlattices with systematically changed coherent strain, thus allowing studying the stress effect on the ferroelectric phase transitions. UV Raman data are supported by the thermodynamic calculations of polarization in superlattices as a function of temperature. The work was done in collaboration with A. Soukiasian, W. Tian, D.G. Schom, Y.L. Li, L.-Q. Chen, X.X. Xi (Pennsylvania State University), A. Bruchhausen, A. Fainstein (Centro Atomico Bariloche & Instituto Balseiro, Argentina), R. S. Katiyar (University of Puerto Rico), A. Cantarero (University of Valencia, Spain), K.J. Choi, D.M. Kim, C.-B. Eom (University of Wisconsin), H.P. Sun, X.Q. Pan (University of Michigan), S.M. Nakhmanson; K.M. Rabe (Rutgers University), Q.X. Jia (Los Alamos National Laboratory).

3:06PM S20.00002 Abnormal retention behavior of Bi3.25La0.75Ti3O12 thin films observed by electrostatic force microscopy1. T.Y. KIM, J.H. LEE, H.R. YOON, Y.J. OH, M.R. CHOI, W.J. OH, Department of Physics and Division of Nanosciences, Ewha Womans University, FERROELECTRICS-AMF TEAM — We report charge retention in c-axis oriented and preferentially (117) oriented ferroelectric thin films. The thin films were observed by electrostatic force microscopy and extended x-ray absorption fine structure, which are useful to interpret the unique retention behaviors in the films. Ramanscattering spectroscopic studies were also used to look into phonon modes of the materials, which are occasionally difficult to understand due to other phases. Surface charges of the films were observed as a function of time in a selected area which consists of a single-poled region and a reverse-poled region. The (117) oriented film shows the extended exponential decay with characteristic scaling exponents, n ~ 1.5. The preferentially c-axis oriented film shows retained behaviors regardless of the poling. Decay and retention mechanisms of the regions are explained by space-charge redistribution and trapping of defects in the films.

3:18PM S20.00003 Chemical Control of Ferroelectric Switching in PbTiO3 Films1. RUEY-VEN WANG, STEPHEN STREIFFER, Center for Nanoscale Materials, Argonne National Laboratory, FAN JIANG, PAUL FUOSS, DILLON FONG, JEFFREY EASTMAN, G. BRIAN STEPHENSON, Materials Science Division, Argonne National Laboratory, KUJTIM LATIFI, CAROL THOMPSON, Department of Physics, Northern Illinois University — Stabilization of monodomain polarization in ultrathin ferroelectric films can be accomplished via surface-adsorbed ions [Fong, D. D. et al., Phys. Rev. Lett. 96, 127601/1-4 (2006)]. Here, we use in-situ grazing-incidence synchrotron x-ray scattering to study the ferroelectric polarization and surface structure of PbTiO3 ferroelectric thin films as a function of vapor environment above the film surface. Coherent PbTiO3 films of 10 nm thickness were grown on conducting SrRuO3 on (001) SrTiO3 substrates. We observe that the polarization direction in the PbTiO3 film can be reversed by changing between oxidizing and reducing conditions. The ferroelectric butterfly loop can be traced out as a function of oxygen partial pressure. Additionally, a new surface reconstruction is observed under reducing conditions.

Work Supported by the U. S. Department of Energy under Contract No. DE-AC02-06CH11357

3:30PM S20.00004 Difference in ferroelectric aging between A-site and B-site acceptor doped BaTiO3 crystals. LIXUE ZHANG, Multi-Disciplinary Materials Research Center, Xi’an Jiaotong University, Xi’an 710049, People’s Republic of China, XIAOBIING REN, Ferroic Physics Group, National Institute for Materials Science, Tsukuba, 305-0047 Ibaraki, Japan — Aging, the time-dependent changing of material properties, has been widely found in acceptor-doped ABO3 ferroelectrics. The origin is usually ascribed to gradual domain stabilization by acceptor-dopant-generated oxygen vacancies. As in ABO3 systems both A-site and B-site acceptor doping can induce oxygen vacancies, they are expected to cause similar aging effect. However, here we report that there exists a significant difference in aging effect between A-site (K-doped) and B-site (Mn-doped) acceptor-doped BaTiO3 crystals. The B-site acceptor doping has much stronger aging effect. This new phenomenon can be fully explained by a semi-quantitative model based on the defect symmetry principle1-4. According to this model, the “strength” of aging is determined by a symmetry-conforming force of the defect symmetry to crystal symmetry. This model may also have potential applications in predicting and understanding the strength of the aging effect in other systems. [1] X. Ren, Nat. Mater., 3:91, 2004; [2] L.X. Zhang, W. Chen and X. Ren, Appl. Phys. Lett., 85:5658, 2004; [3-4] L.X. Zhang and X. Ren, Phys. Rev. B, 71:174108, 2005; Phys. Rev. B 73:094121, 2006.

3:42PM S20.00005 ABSTRACT WITHDRAWN

3:54PM S20.00006 High Speed Nanoscale Ferroelectric Domain Reading and Writing. RAMESH NATH, University of Connecticut, RAMAMOORTHY RAMESH, University of California, Berkeley, BRYAN HUEY, University of Connecticut, UNIVERSITY OF CONNECTICUT COLLABORATION, UNIVERSITY OF CALIFORNIA, BERKELEY COLLABORATION — Piezo Force Microscopy is commonly employed for nanoscale studies of ferroelectric thin films, providing images of local domain orientation and piezoelectric properties. However, applications of PFM to dynamic studies are limited because image acquisition times are long (typically >100 sec.). A recent variation in Atomic Force Microscopy, High Speed Scanning Property Measurements, overcomes this challenge by allowing image frame rates on the order of one second, for image sizes from nanometers to tens of micrometers. For epitaxial thin films of PZT and BiFeO3, domain nucleation and growth is statistically studied at the nanoscale based on hundreds of images acquired at time steps of one second. For uniform films homogenous exponential domain growth is observed, while heterogeneous domain growth is detected at epixaxial PZT grain boundaries. Finally, individual domain reading and writing is achieved at the highest tip speeds reported, beyond 1 centimeter/second, revealing a two-stage relationship between domain size and tip speed discussed experimentally and theoretically.

4:06PM S20.00007 Switching domain dynamics in ferroelectric thin films. ALEXEY GRIGORIEV, University of Wisconsin-Madison, DAL-HYUN DO, REBECCA SICHEL, PAUL EVANS, University of Wisconsin-Madison, BERNHARD ADAMS, ERIC DUFRESNE, Argonne National Laboratory — Polarization switching in ferroelectric materials is governed by the microscopic details of the nucleation and growth of polarization domains. The electric-field dependence of the density of domain nucleation and the domain wall velocity are largely unknown. Using time-resolved x-ray microdiffraction, we have explored the switching dynamics of thin ferroelectric films over a wide range of applied electric fields, starting from the coercive field and ranging up to the maximum field allowed by the thin film capacitors. By separating dynamics of nucleation and domain wall motion we can study the relationship between these two phenomena and their relative contributions to the polarization switching process.
4:18PM S20.00008 Coexistence of polar order and local domain dynamics in ferroelectric SrTi$_{18}$O$_{37}$, ANNETTE BUSSMANN-HOLDER, Max-Planck-Institute for Solid State Research, HELMUT BUETTNER, University of Bayreuth, ALAN BISHOP, Los Alamos National Laboratory — Perovskite oxide ferroelectrics show classical soft mode behaviour typical for the onset of a homogeneous long-range polar state and a displacive phase transition. Besides these long wave length properties, local effects are observed by different probes which reveal that dynamical symmetry breaking already takes place far above the actual instability. It is shown here that displacive mean-field type dynamics can indeed coexist with local dynamical symmetry breaking.

4:30PM S20.00009 Ferroelastic domain dynamics in polydomain, epitaxial BaTiO$_3$ thin films, ANTHONY MEIER, BRUCE WESSELS, Northwestern University — The dynamics of 90° domain switching in polydomain, epitaxial barium titanate thin films were studied using the linear electro-optic effect. Co-planar electrodes were deposited on the film surface and bias was applied in the plane of the film for poling. Upon application of a bias pulse, the E-field driven electro-optic response increased to its saturation value within the 28 ns rise time of the measurement system. Upon removal of the bias pulse, a slow decay of the electro-optic response due to strain-driven relaxation of the ferroelastic domains was observed. Measured relaxation time constants ranged from 5 to 17 ms, exhibiting a power law dependence on the applied E-field amplitude given by $\tau = AE^{n}$ with $n = 0.98-1.23$. X-ray diffraction measurements indicated that under a steady state in-plane bias voltage, the $\alpha$-domain fraction increased while both the $\beta$- and $\gamma$-domain surface normal lattice parameters increased due to the in-plane compressive strains that result from the 90° flipping of $\alpha$-domains. X-ray diffraction measurements after removal of the bias voltage were indistinguishable from those prior to application of the bias voltage indicating that the ferroelastic domains had relaxed back to their original state.

4:42PM S20.00010 Ferroelectric domain dynamics under an external field, ANDREW RAPPE, University of Pennsylvania, YOUNG-HAN SHIN, POSTECH, South Korea, ILYA GRINBERG, I-WEI CHEN, University of Pennsylvania — Ferroelectric oxides with the perovskite structure are promising materials for nonvolatile random access computer memories. Pb$_{1-x}$Ti$_x$O$_3$ is currently used for this purpose. In these materials, storage of a bit involves the reorientation of polarization, or the movement of a ferroelectric domain wall. However, the intrinsic properties of the polarization by experiments or computations. In this talk, I will show how this problem can be studied with a multi-scale approach. First, an interatomic potential is parameterized to first-principles calculations, and molecular dynamics (MD) simulations are performed. Second, stochastic Monte Carlo simulations are conducted, with nucleation and growth rates extracted from the MD simulations. For PbTiO$_3$, we find that while the overall domain-wall speed from our calculation is in good agreement with the experiments, the size of the critical nucleus is much smaller than predicted from the Miller-Weinreich model. We think that this discrepancy can be explained by a diffuse-boundary model and by the fact that the overall wall motion is controlled by both the nucleation and growth processes.

4:54PM S20.00011 Ferroelectric instabilities in CaTiO$_3$ nanoparticles from first principles, SHEN LI, KARIN RABE, Department of Physics and Astronomy, Rutgers the State University of New Jersey, Piscataway, NJ 08854, USA — Ferroelectric instabilities of nanoparticles are expected to be markedly different from those of the bulk material. In many cases, ferroelectricity could be weakened or suppressed, although there is no clear reason why this should always be the case. Previous first-principles studies have shown that in bulk cubic CaTiO$_3$, the polar instability is suppressed by the stronger oxygen octahedron-rotational instabilities, yielding a nonpolar ground state. To investigate the possibility that the nanoparticle configuration could weaken or eliminate the octahedron rotation, we performed first-principles calculations for a single-unit-cell cluster, containing one oxygen octahedron, using a real-space pseudopotential density-functional-theory method (PARSEC). For an electrically isolated cluster, the symmetric nonpolar state is found to be stable. However, if the depolarization field produced by a polar distortion of the cluster is screened, a lower-symmetry polar distorted structure becomes more favorable, so that the cluster can be considered ferroelectric. Our results are consistent with the recent findings regarding the central importance of compensation of the depolarization field in the ferroelectricity of perovskite oxide thin films and nanostructures.

5:06PM S20.00012 A single electric relaxation time in Ba$_{1-x}$Sr$_x$TiO$_3$ nanoparticles at low temperatures, LIYUAN ZHANG, JUN ZHOU, ZHONGLIN WANG, DRAGOMIR DAVIDOVIC, Georgia Institute of Technology — It is shown that the dielectric response of Ba$_{0.77}$Sr$_{0.23}$TiO$_3$ nanoparticles at temperatures below 200K has a frequency and temperature dependence in agreement with the Debye theory with a single relaxation time, which exhibits the Arrhenius law. By contrast, at temperature above 210K the dielectric response exhibits broad range of relaxation times characteristic of relaxor-ferroelectrics. We suggest that the single relaxation time at low temperature indicates frustrated ferroelectricity, analogous to frustrated antiferromagnetism.

5:18PM S20.00013 Size Effect on Ferroelectric Transitions in Nanograin Barium Titanate Polycrystals, I-WEI CHEN, YUDI WANG, University of Pennsylvania, TIEYU SUN, XIAOHUI WANG, Tsinghua University — Data of dielectric constants and polarization of <100 nm BaTiO$_3$ are now available which allows a definitive assessment of the origin of the size effect in these ceramics of multiple polarization transitions. There are three effects to be considered. First, when the grain size is below 500 nm, the ferroelectric behaviour is not accompanied by the formation of multiple domain walls, implicating a large residual stress that causes an increase in the temperatures of subsequent tetragonal/orthorhombic and orthorhombic/rhombohedral transitions. Second, when the grain size of BaTiO$_3$ is below 50 nm, screening of grain boundary charge due to defect segregation is ineffective, implicating a large internal field even above $T_c$. Such a field shifts the temperatures of different transitions differently, favoring the phase of a larger polarization. Third, the dead layer at the grain boundary that clamps the polarization is significant when the grain size decreases to a few nm. It uniformly lowers all the transitions by the same temperature. These effects on transition temperatures and dielectric constant will be compared with the experimental data to assess their relative importance.

Wednesday, March 7, 2007 2:30PM - 5:30PM
Session S27 DMP DCOMP: Focus Session: Computational Nanoscience VI - Nanowires Colorado Convention Center 301

2:30PM S27.00001 The electrostatic and structural properties of GaN nanorods/nanowires from first-principles, M.-H. TSAI, Z.-F. JHANG, J.-Y. JIANG, Y.-H. TANG, L.W. TU, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan — The first-principles calculation has revealed that the GaN nanorod has a greatly enhanced dipole moment per area relative to that of a film, which in conjunction with the geometry effect suggests that the top surface of the GaN nanorod has a greater electrostatic attraction for gas-phase Ga and N source species than the film surface during epitaxial growth of GaN, so that nanorods grow much faster than the film. This electrostatic effect may explain the growth of nanorods protruding high above the film surface. The first-principles molecular-dynamics calculation shows that the average Ga-N bond length of the GaN nanowire decreases with the decrease of the diameter of the nanowire, which demonstrates a surface tension effect. This trend can be expected to be the same for the experimentally grown nanorods, because the physical origin that drives this contraction, namely the surface tension, is the same. Thus, the bond-length result may explain the experimentally observed blue shift of the cathodoluminescence emission.

1Supported by the National Science Council of Taiwan (Contract numbers: NSC 94-2120-M-110-002 and 93-2122-M-110-015).
2:42PM S27.00002 The electronic structure of radial p-n junction silicon nanowires. SHAN-HAW CHIOU, Industrial Research Technology Institute, JEFFREY GROSSMAN, U.C. Berkeley — Silicon nanowires with radial p-n junctions have recently been suggested for photovoltaic applications because incident light can be absorbed along the entire length of the wire, while photogenerated carriers only need to diffuse a maximum of one radius to reach the p-n junction. If the differential of the potential is larger than the binding energy of the electron-hole pair and has a range larger than the Bohr radius of electron-hole pair, then the charge separation mechanism will be similar to traditional silicon solar cells. However, in the small-diameter limit, where quantum confinement effects are prominent, both the exciton binding energy and the potential drop will increase, and the p-n junction itself may have a dramatically different character. We present ab initio calculations based on the generalized gradient approximation (GGA) of silicon nanowires with 2-3 nm diameter in the [111] growth direction. A radial p-n junction was formed by symmetrically doping boron and phosphorus at the same vertical level along the axis of the nanowire. The competition between the slope and character of the radial electronic potential and the exciton binding energy will be presented in the context of a charge separation mechanism.

2:54PM S27.00003 Equilibrium charge and potential distribution of a surrounding-gate silicon nanowire in the LDA approximation. , BART SORREE, WIM MAGNUS, GEOFFREY POURTOIS, STEVEN COMPERNOLLE, IMEC. Kapeldreef 75, B-3001 Leuven, Belgium, REM TEAM — The equilibrium charge and potential distribution of a silicon nanowire is obtained from a Poisson-Schrödinger solver in the local density approximation (LDA). The cylindrical nanowire consists of heavily doped source and drain regions and the channel region is surrounded by a metallic gate. We have studied different cases where the low dimensionality of the wire has a profound effect on the equilibrium charge and electrostatic potential of the gated wire for different gate voltages. Our calculations show that for short channel lengths the built-in potential is significantly lowered and for small diameters volume inversion occurs. We discuss the possible implications for device performance of these low dimensional effects.

3:06PM S27.00004 Structural and Electronic Properties of Silicon Carbide Nanowires¹, SANGUO SHEN, M. YU, C. LEAHY, C.S. JAYANTHI, S.Y. WU, University of Louisville — We have studied the structural and electronic properties of SiC nanowires (NWs) of different diameters (1 nm < d < 7 nm) and shapes (e.g., hexagonal, round, and rhombohedral cross-sections) for wires oriented along <100>, <011>, <111> (cut from the 3C-bulk), and <0001> directions (cut from 2H-, 4H-, or 6H- bulk). A supercell is set-up for each of the above orientations. We relaxed the structures using the state-of-the-art semi-empirical molecular dynamics scheme as described in Ref. [1]. The main results of our findings are: (i) Among the different shapes investigated, NWs with hexagonal morphology are the most stable structures, (ii) Among the hexagonal NWs, those cut from 2H-SiC bulk structures were found to be the most stable ones in the diameter range investigated. They exhibit very weak surface relaxations, and were found to exhibit semiconductor characteristics, (iii) On the other hand, NWs cut from 3C-, 4H-, and 6H- bulk structures exhibit strong facet reconstructions and were found to have metallic characteristics. These results are in agreement with DFT-based ab-initio calculations for small diameter NWs up to 3 nm. [1] Leahy et al. Phys. Rev. B74, 155408 (2006).

¹Sources of funding: KSEF and DoE/EPSCoR.

3:18PM S27.00005 Novel polyicosahedral Si nanowire: A molecular-dynamics study. , KENGO NISHIO, TETSUYA MORISHITA, WATARU SHINODA, MASUHIRO MIKAMI, Research Institute for Computational Sciences, National Institute of Advanced Industrial Science & Technology. Japan — A novel polyicosahedral nanowire, which is composed of linked icosahedral Si nanodots is spontaneously formed in a series of annealing molecular dynamics simulations of liquid Si inside a nanopore of 1.36 nm in diameter[1]. The polyicosahedral Si nanowire is stable even in a vacuum up to about 77% of the melting temperature of bulk Si. Our structural energy calculations reveal that the polyicosahedral nanowire is energetically advantageous over the pentagonal one for a wire whose diameter is less than 6.02 nm, though the latter has been recently proposed as the lowest energy wire. These results suggest the possibility of the formation of a new stable polyicosahedral Si nanowire. [1] J. Chem. Phys. 125, 074712 (2006).

3:30PM S27.00006 Investigation of surface reconstructions in [110] Ge nano-wires.¹, JIAXIN HAN, SCOTT BECKMAN, JAMES CHELIKOWSKY, University of Texas — It is anticipated that nano-structures will lead to the development of novel optical devices. It is known that quantum confinement transforms indirect band-gap crystals into direct band gap nano-structures. Although it is predicted that Ge [110] nano-wires will have a direct band gap, the optical absorption spectra has yet to be measured for free standing Ge nano-wires. Recent calculations have focused on investigating the HOMO-LUMO gap in hydrogenated Ge nano-wires. (1) This surface passivation technique negates surface states, which are suspected to be the primary recombination mechanism in these Ge nano-structures. Here we investigate the surface reconstructions of [110] Ge nano-wires using the real-space density functional theory formalism encoded in the PARSEC software. (2) The structure and electronic states associated with wires as large as 3 nm in diameter have been calculated. Simulated annealing is used to identify the minimum energy structure out of the many possible reconstructions. (1) S. P. Beckman, Jiaxin Han, and James R. Chelikowsky. Phys. Rev. B. 74, 165314 (2006). (2) http://www.ices.utexas.edu/parsec/

¹Supported by the National Science Foundation under DMR-0551195 and by the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760.

3:42PM S27.00007 Ab initio computations of structural and electronic properties of doped and undoped Ge nanowires , D. MEDABOINA, V. GADE, Department of EECS, S. K. R. PATIL, Department of MIME, S. V. KHARE¹, Department of Physics, University of Toledo, OH 43606 — We report results of structural and electronic properties of hydrogen passivated doped and undoped Ge nanowires along [100], [110] and [111] growth directions using density functional theory in the local density approximation (LDA). Cross-sections of nanowires with diameters d > 2.0 nm are faceted reflecting the crystal symmetry about their axis. Nanowires along [100] direction with d below (above) 1.5 nm are found to be direct (indirect) band gap (Eg) semiconductors. Nanowires along [110] have direct Eg for d > 1.0 nm. Nanowires along [111] have indirect Eg for d > 1.0 nm. The magnitude of Eg increases as the wire diameter decreases with values as high as 4.3 eV for a [100] wire with d = 0.41 nm. For a fixed diameter d [100] > Eg [111] > Eg [110] . Doping with P or B did not have a significant effect on the valence and conduction band dispersions.

¹Correspondence: khare@physics.utoledo.edu
of the conductance oscillation requires a first-principles calculation based upon a realistic structure of the wire and the leads. However, little is known about their electronic and optical properties. Here we investigate the electronic structures and optical properties of GaN and ZnO [0001] NWs by using the highly precise full-potential linearized augmented plane wave (FLAPW) method. Our calculations demonstrate that the band gap energy of both the unpassivated and passivated NWs becomes large compared with the bulk energy gap due to quantum confinement effects; surface states crucially affect the electronic structure of unpassivated NWs. Further, we find peculiar features of their dielectric functions that exhibit strong anisotropy in the calculated optical properties. Work supported by the U.S. NSF (through its MRSEC Program at NU).

1Zong et al., Nano Lett. 3, 343 (2003); Ng et al., APL 82, 2023 (2003)
2Akiyama et al., JAP 45, L275 (2006); PRB 73, 235308 (2006)

4:06PM S27.00009 DFT Study of ZnO Nanowire with Wurtzite (0001) Structure . XIAO SHEN, PHILIP B. ALLEN, Stony Brook University, MARK R. PEDERSON, Naval Research Laboratory, JIN-CHENG ZHENG, JAMES W. DAVENPORT, JAMES T. MUCKERMAN, Brookhaven National Laboratory — The most commonly reported ZnO nanowires have the (0001) wurtzite growth axis. We report two first-principles calculations using density-functional theory (DFT) for a small model nanowire with diameter 0.9 nm, containing 26 atoms in one periodic repeat unit cell, arranged as a fragment of a wurtzite (0001) crystal. One calculation is done on an infinite wire and the other on a truncated piece. The two calculations show excellent agreement. In both calculations, the atomic coordinates were relaxed to the nearest stable minimum. The exposed (1100) surfaces resemble closely the relaxed surface found in bulk. Our calculation shows that the c axis has a ~2% elongational strain. We also compute the change of the Young’s modulus relative to the bulk, and compare our prediction with experiment. The electrical polarization of this non-centrosymmetric nanowire will be discussed, and also the assignment of a rotational quantum number m to the Bloch band states.


4:18PM S27.00010 Capillary stability of nanowires in the presence of dislocations1, MARK JHON, DARYL CHRZAN, ANDREAS GLAESER, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratories — Nanometer scale structures are often unstable with respect to capillary forces. For instance, wires may be susceptible to a peeling (Rayleigh) instability or to coarsening. A simple continuum theory is presented that predicts that sufficiently small second phase wires formed around dislocations are stable to both forms of structural instability. The elastic interaction is found to balance the effects of surface energy. Infinitesimally small perturbations to an isolated wire are found to decay for wires smaller than a critical size. For an ensemble of wires smaller than the critical size, a driving force is found for inverse coarsening. These results imply that thermally stable nanometer-scale wires can be produced.

1MHJ gratefully acknowledges a fellowship from the Intel Foundation. This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

4:30PM S27.00011 Stability of conductance oscillations in monatomic sodium wires , PETR KHOMYAKOV, GEERT BROCKS, CMS-TNW, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands — We study the stability of conductance oscillations in monatomic sodium wires with respect to structural variations. The geometry, the electronic structure and the electronic potential of sodium wires suspended between two sodium electrodes are obtained from self-consistent density functional theory calculations. The conductance is calculated using the Landauer-Buttiker formalism and the mode-matching technique as formulated recently in a real-space finite-difference scheme [PRB 70, 195402 (2004)]. We find a regular even-odd conductance oscillation as a function of the wire length, where wires comprising an odd number of atoms have a conductance close to the quantum unit, and even-numbered wires have a lower conductance. The conductance of odd-numbered wires is stable with respect to geometry changes in the wire or in the contacts between the wire and the electrodes; the conductance of even-numbered wires is more sensitive. Geometry changes affect the spacing and widths of the wire resonances. In the case of odd-numbered wires the transmission is on-resonance, and hardly affected by the

4:42PM S27.00012 Quantum and classical simulations of nanowire self-assembly . ZHIGANG WU, JEFFREY GROSSMAN, University of California, Berkeley — The ability to control the synthesis of nanostructures such as nanowires and nanotubes is crucial to the success of next-generation nanotechnology devices. One promising approach for efficiently controlling fabrication is to functionalize nanoscale building blocks such that they will self-assemble under the appropriate conditions. We employ a combination of ab initio total energy calculations, classical molecular dynamics (MD), and classical Monte Carlo (MC) calculations to investigate the possible self-assembly of nanoscale objects into chains and wires. The ab initio calculations provide key information regarding selective chemical functionalization for end-to-end attraction and the subtle interplay of the energy landscape, which is then used to fit classical potentials. Using these potentials, MD simulations are carried out to predict short-time (i.e., ps and ns timescales) dynamical properties of nanoparticle assembly as a function of particle shape, chemical functionalization, and temperature. Finally, both static and dynamical data from these calculations are used in MC simulations to predict large time- and length-scale assembly under a variety of synthesis conditions. Our results suggest a new technique for bringing nanoscale objects together to form ordered, ultra high-aspect ratio nanowires.

4:54PM S27.00013 Molecular Simulation of Size-Dependent Properties of Polymeric Nanofibers . SEZEN CURGUL, GREG RUTLEDGE, KRYSTYN VANVLIET, MIT — Materials with nanometer dimensions have been shown experimentally to exhibit size dependent properties. Polymeric nanofibers, in particular, are of interest because of their several value added applications such as medical, filtration, barrier, wipes, personal care, composite, garments, insulation, and energy storage. We report here the results of molecular dynamics (MD) simulations of polymer nanofibers using LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator). To date, we have simulated fibers comprised of chains that mimic the prototypical polymer polyethylene, with chain lengths ranging between C50 and C300. These nanofibers have diameters in the range 1.86-16.2 nm. The fibers have been analyzed for signature of size dependent behavior in their structural and dynamical properties. In these fibers, mass and energy density profiles are similar and they have constant bulk-like values at the center of the fiber, for sufficiently large diameter fibers. The surface layer thickness shows little dependence on the fiber size. The interfacial excess energy increases with decreasing fiber size for fibers below 5 nm in diameter. The chains at the surface show preferred conformations and orientations that are significantly different than chains at the center of the nanofiber.
the capacitance measured directly. Transport model and calculation fit very well with the experiment data. In addition, the mobility of the SWNT FETs at room temperature is also extracted by bias is clearly observed, due to the large geometric capacitance comparable to or even larger than the quantum capacitance of the SWNT. Theoretical quantum (functionalization of single walled carbon nonotubes (SWNTs) with ploy-T DNA molecules, which can impart functional groups of sufficient density and stability to improve the ultimate vertical scaling limit of carbon nanotube field effect transistors (FETs) and reliably achieve S$\sim 200aF$). Of the SWNT FET has been successfully measured directly, using a special technique. The quantum capacitance oscillation with top gate voltage of the nanowire breaking process, but at room temperature silver and copper contacts adopt a zigzag structure (as predicted by first principles calculations) that becomes unstable. We found that the stability and the average number of atoms forming these chains depend on the metal species, a fact that can be explained in terms of the population of d-orbitals along the chains. Besides to clarify the controversy in the literature on the formation of these chains in 3d and 4d metals, our findings give insights on the advantages and limitations of detecting them through conductance measurements.

Wednesday, March 7, 2007 2:30PM - 5:30PM — Session S28 DMP: Focus Session: Carbon Nanotubes: Devices Colorado Convention Center 302

2:30PM S28.00001 Electrical Contacts to Nanotubes and Nanowires. FRANÇOIS LÉONARD, Sandia National Laboratories — Electrical contacts play a key role in electronics. As new materials such as nanotubes and nanowires are explored for nanoelectronics, the fundamental aspects of electrical contacts need to be re-examined due to the unique properties of these nanostructures. In this talk, recent theoretical and modeling results will be presented on the properties of electrical contacts to carbon nanotubes and nanowires. For these quasi-one dimensional (Q1D) structures, side contact with the metal only leads to weak band realignment, in contrast with bulk metal-semiconductor contacts. Schottky barriers are much reduced compared with the bulk limit, and should facilitate the formation of good contacts. However, the conventional strategy of heavily doping the semiconductor to obtain Ohmic contacts breaks down as the nanowire diameter is reduced. The issue of Fermi level pinning will also be addressed, and I will discuss how the unique density of states of Q1D structures makes them less sensitive to this effect. The results agree with recent experimental work, and should apply to a broad range of Q1D materials.

2:30PM S28.00002 Tunable contact barriers at single wall carbon nanotube/silicon heterojunctions . ZHUANGCHUN WU, BO LIU, ANDREW G. RINZLER, University of Florida — Due to their prevalence in modern electronic devices understanding contact barriers at metal-semiconductor junctions remains an important area of research. However, due to the sensitivity of such junctions to surface states modified by parameters like the semiconductor surface preparation, the type of metal used, and its method of deposition, this remains an area rich in complications (viz. Fermi-level pinning). Single wall carbon nanotubes (SWNTs), by virtue of their highly passivated side-walls, provide an opportunity to reduce this complexity by their lack of covalent interaction with the semiconductors on which they can be deposited. The porosity of nanotube film contacts provides further opportunities not available with contiguous metal contacts. We describe experiments in modulating the contact barrier between SWNT/Si heterojunctions using an ionic liquid gate. Modest gate voltages are shown to modify the contact barriers modulating the current across the junction by a factor of 300.

3:06PM S28.00003 Encapsulation of floating carbon nanotubes in SiO$_2$. LEONIDAS TSETSERIS, SOKRATES PANTELIDES, Vanderbilt University — In many applications of carbon nanotubes (CNT), it is desirable to have them embedded in a dielectric such as SiO$_2$, without significantly impacting their electronic properties. Here we study the CNT-SiO$_2$ interface of an embedded CNT using first-principles calculations. Our results suggest that a carbon nanotube can be incorporated inside a SiO$_2$ matrix that nucleates around it through the formation of Si-O-C bridges. The large distortion associated with the formation of these bridges can be alleviated by hydrogenation of the composite. Introduction of hydrogen in the vicinity of the bridges leads to their elimination, whereby the nanotube loses its anchoring to the matrix and it floats. For CNTs of suitable diameter, the final floating structure has electronic properties very close to the structure in vacuum. Overall, our results provide atomic-scale information that is relevant to a broad range of applications using embedded or adsorbed nanotubes, for example, sensors, electronics, actuators, and CNT coatings. This work was supported in part by DOE Grant DEFG0203ER46096.

3:30PM S28.00004 Carbon Nanotube FET Mixers and High Frequency Applications , ZHAOHUI ZHONG, Center for Nanoscale Systems, Cornell University, Ithaca, 14850; XIJIAN ZHOU, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, 14850; PAUL MCEUEN, Center for Nanoscale Systems; Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, 14850 — We have investigated the high magnetic electrical properties of single-walled carbon nanotube field effect transistors by operating the devices as microwave mixers. The mixing current amplitude depends linearly on the transconductance and quadratically on the applied AC voltage. On devices with insulating substrates, the response is approximately independent of frequency up to 40 GHz. Two applications of these high frequency-operation carbon nanotube FET mixers will be discussed: the detection of terahertz electrical pulses and nanoscale dielectric spectroscopy of liquids.

5:06PM S27.00014 Raman Antenna Effect in Semiconducting Nanowires. , GUGANG CHENG, QIHUA XIONG, PETER EKLUND, Department of Physics, The Pennsylvania State University — A novel Raman antenna effect has been observed in Raman scattering experiments recently carried out on individual GaP nanowires [1]. The Raman antenna effect is perfectly general and should appear in all semiconducting nanowires. It is characterized by an anomalous increase in the Raman cross section for scattering from LO or TO phonons when the electric field of the incident laser beam is parallel to the nanowire axis. We demonstrate that the explanation for the effect lies in the polarization dependence of the Mie scattering from the nanowire and the concomitant polarization-dependent electric field set up inside the wire. Our analysis involves calculations of the internal electric field using the discrete dipole approximation (DDA). We find that the Raman antenna effect happens only for nanowire diameters d<\lambda/4, where \lambda is the excitation laser wavelength. Our calculations are found in good agreement with recent experimental results for scattering from individual GaP nanowires. [1] Q. Xiong, G. Chen, G. D. Mahan, P. C. Eklund, in preparation, 2006.

5:18PM S27.00015 Structure and stability of suspended monatomic metal chains , ANWAR HASMY, NIST, Gaithersburg MD & Inset Group, PMUSA, Richmond VA, LUIS RINCON, NIST, Gaithersburg MD & ULA, Venezuela, RAIZA HERNANDEZ, IVIC, Venezuela, MANUEL MARQUEZ, VLADIMIRO MUJICA, NIST, Gaithersburg MD & Inset group, PMUSA, Richmond VA, CARLOS GONZALEZ, NIST, Gaithersburg MD — Since the spectacular achievement of the ultimately thin wire (a suspended monatomic gold chain) little progress has been made on the origin and the ubiquity of this phenomenon. Here we report a systematic quantum study on breaking monovalent metal nanowires through tight-binding molecular dynamics simulations. We show that at low temperature (4 K) gold, silver and copper can form linear and stable suspended monatomic chains at the late stage of the nanowire breaking process, but at room temperature silver and copper chains adopt a zigzag structure (as predicted by first principles calculations) that becomes unstable. We found that the stability and the average number of atoms forming these chains depend on the metal species, a fact that can be explained in terms of the population of d-orbitals along the chains. Besides to clarify the controversy in the literature on the formation of these chains in 3d and 4d metals, our findings give insights on the advantages and limitations of detecting them through conductance measurements.

3:30PM S28.00004 Carbon Nanotube FET Mixers and High Frequency Applications , ZHAOHUI ZHONG, Center for Nanoscale Systems, Cornell University, Ithaca, 14850; XIJIAN ZHOU, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, 14850; PAUL MCEUEN, Center for Nanoscale Systems; Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, 14850 — We have investigated the high magnetic electrical properties of single-walled carbon nanotube field effect transistors by operating the devices as microwave mixers. The mixing current amplitude depends linearly on the transconductance and quadratically on the applied AC voltage. On devices with insulating substrates, the response is approximately independent of frequency up to 40 GHz. Two applications of these high frequency-operation carbon nanotube FET mixers will be discussed: the detection of terahertz electrical pulses and nanoscale dielectric spectroscopy of liquids.

4:32PM S28.00005 Capacitance Measurement for FETs of Individual SWNTs with Altra-Thin ALD High-k Dielectric , YUERUI LU, RYAN TU, YOSHIO NISHI, HONGJIE DAI, Stanford University — Recently, we have been able to approach the ultimate vertical scaling limit of carbon nanotube field effect transistors (FETs) and reliably achieve 5 ~ 60 mV/decade at room temperature, by non-cova lent functionalization of single walled carbon nanotubes (SWNTs) with poly-T DNA molecules, which can impart functional groups of sufficient density and stability for uniform and conformal ALD of high-k dielectrics (HfO$_2$) with thickness down to 2-3 nm on SWNTs. Moreover, very small top gate stack capacitance (~200aF) of the SWNT FET has been successfully measured directly, using a special technique. The quantum capacitance oscillation with top gate voltage bias is clearly observed, due to the large geometric capacitance comparable to or even larger than the quantum capacitance of the SWNT. Theoretical quantum transport model and calculation fit very well with the experiment data. In addition, the mobility of the SWNT FETs at room temperature is also extracted by the capacitance measured directly.
Single-walled carbon nanotubes (SWNTs) are promising materials for future high performance and nano-electronics due to their high performance of SWNT field effect transistors (FETs) such as Ohmic contact, nearly ballistic transport and ideal switching when integrated with thin high-κ -materials. Yet the ideal structure for SWNT transistors is still unclear due to non-ideal behaviors when transistor size is scaled down. Recently, PIN structure is proposed as an ultimate structure for SWNT-FETs on a single device level. In this work, SWNT-FETs with n- and p- doped source and drain and ultra thin high-κ gate dielectrics is first experimentally fabricated and characterized. This novel tunneling transistor structure is based on quantum mechanical band-to-band tunneling current between conduction and valence band of semiconducting SWNTs. The combination of these techniques allows the charge states involved in transport through the nanotube to be directly probed. The spectroscopy measurements show peaks due to Coulomb blockade, which split and change energy as a function of the source-drain voltage across the nanotube. These splitting peaks track the Fermi level of the source and drain electrodes. With our combined measurement technique, we are able to show that these peaks in the spectroscopy are correlated with changes in the source-drain current. This demonstrates that the states identified by the spectroscopy measurement are the same delocalized states involved in transport through the nanotube. Unexpectedly, the strength of these spectroscopy peaks depends on position along the nanotube.

We performed the transport measurement through single-walled carbon nanotubes (SWCNT). The transport characteristic changes dramatically when the metal electrodes of the devices switch from normal state to Coulomb blockade, which split and change energy as a function of the source-drain voltage across the nanotube. Only those nanotube devices with room temperature resistance below 15kΩ were examined. The differential contact is highly transparent, individual SWCNT can carry a supercurrent by means of proximity effect. We developed a technique to perform simultaneous electrical transport and scanning tunneling spectroscopy measurements on carbon nanotubes. The combination of these two techniques allows for conduction and valence band of semiconducting SWNT to be directly probed. The spectroscopy measurements show peaks due to Coulomb blockade, which split and change energy as a function of the source-drain voltage across the nanotube. These splitting peaks track the Fermi level of the source and drain electrodes. With our combined measurement technique, we are able to show that these peaks in the spectroscopy are correlated with changes in the source-drain current. This demonstrates that the states identified by the spectroscopy measurement are the same delocalized states involved in transport through the nanotube. Unexpectedly, the strength of these spectroscopy peaks depends on position along the nanotube.

We have developed a technique to perform simultaneous electrical transport and scanning tunneling spectroscopy measurements on carbon nanotubes. The combination of these two techniques allows for conduction and valence band of semiconducting SWNT to be directly probed. The spectroscopy measurements show peaks due to Coulomb blockade, which split and change energy as a function of the source-drain voltage across the nanotube. These splitting peaks track the Fermi level of the source and drain electrodes. With our combined measurement technique, we are able to show that these peaks in the spectroscopy are correlated with changes in the source-drain current. This demonstrates that the states identified by the spectroscopy measurement are the same delocalized states involved in transport through the nanotube. Unexpectedly, the strength of these spectroscopy peaks depends on position along the nanotube.

Moreover, we observed a pronounced zero-bias conductance peak, which is tunable by gate voltage. Such conductance peak is attributed to multiple Andreev conductance of S-CNT-S junction showed periodic oscillations as a function of both drain-source and gate voltage, a signature of Fabry-Perot interference. S-CNT-S type Josephson junction at 260mK. The work is supported by the Office of Naval Research (GB060468).
Remote phonon scattering in NT field effect transistors. ALEXEY G. PETROV, Ioffe Institute, SLAVA V. ROTKIN, Lehigh University — We developed a theory of the remote phonon (RP) scattering for the hot charge carriers in nanotube (NT) field effect devices that use polar dielectric substrates, such as SiO2 or high-kappa materials [JETP Lett 84, 156, 2006]. We calculated the effect of this novel scattering mechanism on the NT conductivity. We stress that in contrast to any other scattering mechanisms studied earlier the RP scattering allows to transfer the excess energy of the hot carriers directly to the substrate (not through the NT lattice). The macroscopic substrate has no limitation of a finite thermal capacity as a single NT has. Therefore, our RP scattering mechanism is advantageous for the high power NT devices, especially when aggressively scaling down the size and scaling up the operational frequency. We obtained a scattering time within a self-consistent quantum mechanical approach for inter- and intra-subband transitions in semiconductor and metallic NTs. The intra-subband transitions with forward scattering are shown to prevail over the inter-subband transitions as well as the backward scattering. We obtained the polaronic effects by solving for the electron energy and life-time self-consistently. We found the upper limit of the spacing between the NT and the polar dielectric for the RP scattering to become ineffective, which is approximately 40 nm for the quartz substrate.

Wednesday, March 7, 2007 2:30PM - 5:30PM
Session S39 FIAP DMP: Focus Session: Hydrogen Storage IV Colorado Convention Center 502

Hydrides from Density Functional Theory. LOUIS HECTOR JR., JAN HERBST, GM Research and Development Center, Warren MI 48090-9055 — Thermodynamic and vibrational properties of La(TM)Hx (TM = Co, Ni, Ti) and their antecedent intermetallics are discussed. Enthalpies of formation, ΔH, are computed with the plane wave density functional method implemented in the Vienna Ab Initio Simulation Package (VASP). All electron projector-augmented wave potentials based upon the generalized gradient approximation are used for the elemental constituents. With suitable supercells, the zero point and finite temperature contributions to ΔH are computed with the direct phonon method using VASP as the computational engine. Phonon dispersion curves and total phonon density of states are examined for soft modes in each compound and important vibrational modes are identified. The computed vibrational spectra for LaCo2 and LaCo2H8 reveal new information on their crystal structures.

Hydrogen Bonding in CaSiH(D)1+x: Is there Covalent Character?1, T.J. UDOVIC, H. WU, W. ZHOU, J. J. RUSH, T. YILDIRIM, NIST Center for Neutron Research — We report here our neutron powder diffraction and neutron vibrational spectroscopy study of CaSiH(D)1+x, along with first-principles calculations, which reveal the hydrogen structural arrangements and bonding in this novel alloy hydride. Both structural and spectroscopic results show that, for x > 0, H(D) atoms start occupying a Ca3Si interstitial site. The corresponding Si-H(D) bond length is determined to be 1.02 Å, fully 0.24 Å larger than predicted by theory. Here we discuss in detail our neutron spectroscopic measurements, which are also generally at odds with strongly covalent Si-H bonding in CaSiH1+x that such calculations suggest. These results may have implications for a number of ongoing studies of metal-hydrogen systems destabilized by Si alloying.

Structure and Bonding in Destabilized Metal Hydrides for Hydrogen Storage. HUI WU, University of Maryland and NIST Center for Neutron Research — Light-metal hydrides possess high hydrogen-storage capacities (> 5 wt.%), but their utility is generally compromised by high thermal stability, rather slow absorption kinetics, and/or problems with reversibility for hydrogen absorption/desorption cycling. There has been great emphasis, particularly in recent years, on attempts to destabilize and otherwise improve the properties of these hydrides by alloying with Si and other elements. We describe here the study of lithium and calcium hydrides alloyed with Si and Ge using ball-milling techniques. The details of the structure and bonding of the Li/Si/H(D), Li/Ge/H(D) and Ca/Si/H(D) systems have been revealed through a combination of neutron and x-ray diffraction, neutron spectroscopy and first-principles calculations. We report the discovery of several new hydride phases, the nature of Si-H bonding in these hydride systems and the effects of amorphization in the Ca/Si/H alloys. The implications of our results for future investigations will be discussed.

Hydrogen In-Situ Hydriding/Dehydriding. STEPHEN KELLY, RAJ KELKAR, HERMIONE GIFFARD, BRUCE CLEMENS, Stanford University — Magnesium is an attractive material for hydrogen storage because it stores an appreciable amount of hydroge (7.6 wt.%) as magnesium hydride (MgH2), is abundant in the earth’s crust and is relatively inexpensive. Understanding of the structural changes and associated kinetics for the magnesium/magnesium hydride phase transition is crucial to engineering practical metal hydride hydrogen storage materials involving magnesium. A thin film architecture allows us to deposit and analyze precisely controlled structures in order to gain insight into the kinetic mechanisms present in the phase change. Using UHV sputter deposition onto a variety of substrates we have grown Mg thin films with varying degrees of structural texture and orientation. Using x-ray diffraction with in-situ sample heating we see evidence for a solid phase epitaxial (SPE) regrowth mechanism for the Mg regrowing from the MgH2 in epitaxial Mg thin films and observe kinetic differences for the discharging of films with different Mg orientations (Mg c-axis in/out of the sample plane). We also determined the crystallographic orientation correlation for the Mg to MgH2 transition in our epitaxial thin films. Here we also present our recent work examining and analyzing the kinetics for sample charging utilizing a variety of methods.

1This work is supported by the Division of Materials Science, Office of Science, Basic Energy Sciences under contract DE-AC05-00OR22725 and the NSF under DMR-0412231.
Density functional calculations are used to calculate the structural and electronic properties of BaReH$_9$ and to analyze the bonding in this compound. This compound has an exceptionally high H to metal ratio of 4.5. The high coordination of Re in BaReH$_9$ is due to bonding between Re 5d states and states of d-like symmetry formed from combinations of H s orbitals in the H$_3$ cage. This explains the structure of the material, its short bond lengths and other physical properties, such as the high band gap. We compare with results for hypothetical BaMnH$_9$, which we find to have similar bonding and cohesion to the Re compound. This suggests that it may be possible to synthesize (MnH$_x$)$_{3-}$ salts. Depending on the particular cation, such salts may have exceptionally high hydrogen contents, in excess of 10 weight %.

1 Work at ORNL is supported by DOE, DMS&E.

4:18PM S39.00008 Thermodynamic considerations in the synthesis of complex metal hydrides via mechanosynthetic techniques, ASHLEY C. STOWE, POLLY A. BERSETH, ARTHUR JURGENSEN, DONALD ANTON, RAGAÏ Y ZIDAN, Savannah River National Laboratory — Complex metal hydrides have been synthesized for hydrogen storage through a new synthetic technique utilizing high hydrogen overpressure at elevated temperatures (molten state processing). This synthesis technique holds the potential of fusing different known complex hydrides at elevated temperatures and pressures. Two main new species within the complex hydride family, namely hydrogen storage materials, were identified using thermodynamic and kinetic considerations. Novel synthetic complexes were structurally characterized and their hydrogen desorption properties were investigated. The effectiveness of the molten state process will be compared with mechanosynthetic ball milling.

4:30PM S39.00009 Combinatorial thin film deposition and infrared emission characterization of hydrogen storage materials, LEONID BENDERSKY, Materials Science and Engineering Laboratory, NIST, HIROYUKI OGUCHI, University of Maryland, EDWARD HEILWEIL, Physics Laboratory, NIST, DANIEL JOSELL, Materials Science and Engineering Laboratory, NIST — Optimal hydrogen sorption/desorption behavior (temperature, pressure, kinetics) depends on a composition and a microstructural state. Combinatorial thin films provide a wide range of continuously changing compositions and microstructures (amorphous, nanocrystalline, single crystal, multiphases) on a single substrate. In this paper we report preparation and characterization of two systems, Fe$_2$Ti-Fe$_2$Ti$_4$MgNi-Mg on silicon wafers with Pd overlayers. The specimens were prepared by a shutter-controlled multilayer e-beam deposition. After-deposition annealing can create a variety of microstructural states. Both as-deposited and annealed films were fully characterized by SEM, x-ray, and selectively by TEM. Hydrogenation of the films was monitored with an infrared (IR) camera. Changes in the IR emissivity in response to the film hydrogenation and phase transition behavior will be discussed.

4:42PM S39.00010 Hydrogen Fueling via Guanidinum, J. A. VAN VECHTEN, Oregon Sustainable Energy — Three related materials, ammonia (NH$_3$), urea (OCN$_2$H$_4$), and guanidine (C$_3$N$_5$H$_5$) are practicable hydrogen-based fuels that could be produced in the giga-tonne quantities required from air, water, and renewable energy. NH$_3$ has long been established as a fuel for internal combustion engines and can be cracked to H$_2$ for use in fuelcells, but is a gas at STP and extremely toxic, so general use is problematic. Urea and guanidine can easily be converted to NH$_3$ and CO$_2$ by addition of hot water from oxidation of NH$_3$. Both are solids at STP, non-toxic, non-explosive and commonly shipped in plastic bags. The energy density in kWhr/L of guanidine is 4.7 compared with 3.0 for urea, 3.5 for liquid NH$_3$, and 0.8 for H gas in 10,000 psi tanks. The specific energies in kWhr/kg for these materials are respectively 3.58, 2.35, 5.2, and (including the tank) 1.8. Guanidine melts at 50°C and is infinitely soluble in both ethanol and water. 1 http://www.energy.iastate.edu/renewable/biomass/AmoniumMgt06.html

4:54PM S39.00011 Bi-Liquid Hydrogen Generation Using Familiar Materials, JEREMIAH CRONIN, American Physical Society — Greater acceptance of Fuel Cell Power Systems has been greatly constrained due to the lack of a low cost, energy dense, and convenient hydrogen source to fuel these systems. This talk will present a novel bi-liquid approach to resolving current impediments to mobile hydrogen production, and how current R&D is applicable to this bi-liquid approach. The implications of this bi-liquid fueling concept on other primary Fuel Cell subsystems, and an approach to commercial implementation will also be presented. The closing remarks will additionally identify benefits to the nation beyond those normally envisioned in the promise of a hydrogen based economy.

5:06PM S39.00012 Hydrogen clathrate hydrates as a potential hydrogen storage material, DUBRAVKO SABO, JACALYN CLAWSON, SUJAN REMPE, JEFFERY GREATHOUSE, MARCUS MARTIN, KEVIN LEUNG, SAMEER VARMA, RANDALL CYGAN, TODD ALAM, Sandia National Laboratories — Recent synthetic activities involving hydrogen clathrate hydrates raised the prospect of utilizing them as an alternative storage material for hydrogen fuel. The current work is a starting point for future studies of hydrogen occupancy of hydrogen clathrate hydrate and its stability. We present studies of the structural and thermal properties of a hydrogen molecule dissolved in liquid water and their possible implication for hydrogen storage in clathrate hydrates. This is a new species within the family of hydrogen storage materials, and hydrogen contents, in excess of 10 weight %.

1 DOE

5:18PM S39.00013 Clathrate hydrates studied by diffraction and vibrational spectroscopy, TIMOTHY JENKINS, Carnegie Institution of Washington, RUSSELL HEMLEY, Carnegie Institution of Washington, WENDY MAO, Los Alamos National Laboratory, HO-KWANG MAO, BURKHARD MILITZER, VIKTOR STRUZHKIN, Carnegie Institution of Washington — Clathrate hydrate structures are a potentially viable method for hydrogen storage (Mao and Mao 2004). For simple hydrogen-water clathrates, low temperatures (<150 K) or high pressures (>2 kbar) are needed for stability. We investigated, using inelastic neutron spectroscopy, the hydrogen storage character of a clathrate of hydrogen with the addition of tetrahydrofuran as a promoter molecule. The addition of tetrahydrofuran allows the formation of the clathrate structure at elevated temperature and decreased pressure as compared to the hydrogen clathrate (Lee, et al. 2005). In addition we have examined the higher pressure clathrate forms at lower temperature. High pressure diamond anvil work has allowed Raman and x-ray spectroscopy on novel clathrate environments. Analysis of these model compounds will assist in future investigations to additional clathrate compounds.


Wednesday, March 7, 2007 2:30PM - 5:30PM – Session S44 DMP: Focus Session: Optical Properties of Plasmonic Nanostructures Colorado Convention Center 507
2:30PM S44.00001 Au Bowtie Nanostructures for Surface-enhanced Raman Spectroscopy. DANIEL WARD, Department of Physics and Astronomy, Rice University, NATHANIEL GRADY, Department of Electrical and Computer Engineering, Rice University, CARLY LEVIN, Department of Chemistry, Rice University, NAOMI HALAS, Department of Electrical and Computer Engineering, Rice University, DOUGLAS NATelson, Department of Physics and Astronomy, Rice University — Designing nanostructures for surface-enhanced Raman spectroscopy (ERS) is an active area of research because of the potential for chemical sensing with single-molecule sensitivity. We report preliminary ERS measurements on Au bowtie structures with nanometer size interelectrode gaps fabricated by electronbeam lithography. Initial data suggest that the bowtie structures provide a large electromagnetic enhancement for ERS over a small volume, enabling few or single molecule spectroscopy. The local plasmon resonance of the bowtie structure is tunable by varying the width of the gap between the two halves using electromigration. Additionally we report on a multiple bowtie structure that combines several bowtie devices in parallel allowing for the simultaneous electromigration of several devices at once to similar gap sizes.

2:42PM S44.00002 Optical Response of Metal Nanoantennas to Femtosecond Pulses. SUSHMITA BISWAS, Dept of Physics and Astronomy, Univ of Pittsburgh, ALBERT HEBERLE, Dept. of Physics and Astronomy. Dept. of Electrical and Computer Engineering, University of Pittsburgh — Nanoscale metal antennas are promising devices for focusing light down to dimensions much smaller than the wavelength of light. This focusing can lead to strong optical enhancement of the response of single molecules or quantum dots placed in the antenna gap, as well as strong nonlinearities. The optical response of such an antenna, however, is not well understood yet. Here, we will present results of our investigations of the linear and nonlinear optical response of silver nanoscale bowtie antennas to excitation with near-infrared pulses from a femtosecond Ti:sapphire laser. The antennas were fabricated with electron beam lithography and a lift-off process on glass substrates and semiconductor materials. They have lengths of a few hundred nanometers and gaps between 10 and 100 nanometers. We will discuss polarization dependence of the excitation sensitivity, second harmonic generation and other nonlinear effects.

References:

1 NSF-DMR PD 03-1710

2:54PM S44.00003 Two-Photon Vibrational Spectroscopy using local optical fields of gold and silver nanostructures. KATRIN KNEIPP, Harvard Medical School, Wellman Center for Photomedicine, JANINA KNEIPP, Federal Institute for Materials Research and Testing, Berlin, HARALD KNEIPP, Harvard Medical School, Wellman Center for Photomedicine, HARVARD MIT HST TEAM, FEDERAL INSTITUTE FOR MATERIALS RESEARCH AND TESTING, D-12489 BERLIN TEAM, HARVARD MEDICAL SCHOOL, WELLMAN CENTER FOR PHOTOMEDICINE, BOSTON, MA TEAM — Spectroscopic effects can be strongly affected when they take place in the immediate vicinity of metal nanostructures due to coupling to surface plasmons. We introduce a new approach that suggests highly efficient two-photon labels as well as two-photon vibrational spectroscopy for non-destructive chemical probing. The underlying spectroscopic effect is the incoherent inelastic scattering of two photons on the vibrational quantum states performed in the enhanced local optical fields of gold nanoparticles, surface enhanced hyper Raman scattering (SEHRS). We infer effective two-photon cross sections for SEHRS on the order of 10^5 GM, similar or higher than the best known cross sections for two-photon fluorescence. SEHRS combines the advantages of two-photon spectroscopy with the structural information of vibrational spectroscopy, and the high sensitivity and nanometer-scale local confinement of plasmonics-based spectroscopy.

3:06PM S44.00004 Interparticle and Interfacial Effects on Second Harmonic Generation from Gold Nanoparticles. MATTHEW MCMAHON, DAVON FERRARA, RICHARD HAGLUND, Vanderbilt University — We have studied the angular dependence of second-harmonic generation (SHG) from symmetric gold nanoparticles arranged in lithographically fabricated gratings. For example, we have measured the effects of electric-field enhancement on second-harmonic generation by controlling the separation between closely spaced nanoparticles; changing the separation should change the strength of the interaction. Near-field interparticle interactions are observed to have characteristic effects on both the extinction spectra and the second-harmonic signals. Moreover, the substrate plays an important role in the way dipoles and higher-order multipoles contribute to the harmonic radiation. We have computed the dipole and quadrupole contributions in order to fit the measured SHG angular distributions. Theoretically, however, most of the harmonic light should be radiated into the substrate rather than into free space, making waveguiding applications particularly intriguing.

3:18PM S44.00005 Strong Field Enhancement in a Scanning Nanogap for Infrared Imaging of Single Nanoparticles (lambda/1000). JAVIER AIZPURUA, Donostia International Physics Center, San Sebastian, Spain, ANTONIJA CVITKOVIC, NENAD OCELIC, REINHARD GUCKENBERGER, RAINER HILLENBRAND, Max-Planck Institute for Biochemistry, Martinsried, Germany — Far-field infrared analysis of individual nanoparticles has not been possible so far due to the extremely weak scattering cross section of nanosize objects at infrared wavelengths, which is 5 orders of magnitude smaller than at visible wavelengths. Scattering type near-field optical microscopy (s-SNOM) offers nanoscale spatial resolution at IR wavelengths and background-free imaging [1,2]. We investigate theoretically and experimentally the use of strong optical field enhancement in the nanogap formed between the s-SNOM tip and the substrate supporting the particles. We show the key role of the substrate response to obtain strong field enhancement at the scanning gap, and therefore spatially resolve the nanoparticles. We provide clear experimental evidence that for highly reflective substrates, single particles as small as 8 nm can be detected with a mid-IR s-SNOM operating at 10 micrometer wavelength. [1] F Keilmann and R. Hillenbrand, Phil. Trans. Roy. Soc. A 362, 787 (2004). [2] A. Cvitkovic et al., Phys. Rev. Lett. 97, 060801 (2006).

3:30PM S44.00006 Enhanced thermal emission from individual antenna-like nanoheaters. SNORRI INGVARSSON, Science Institute, University of Iceland, JAMES A. LACEY, HENDRIK F. HAMANN, IBM T.J. Watson Research Center, Yorktown Heights, NY 10598 — We report polarization-sensitive, thermal radiation measurements of individual, antenna-like, thin film Platinum nanoheaters. These heaters confine the lateral extent of the heated area to dimensions smaller or comparable to the emission wavelengths. We investigate the polarization patterns of the far-field radiation from individual nanoheaters as a function of length and width. For very long and narrow heater structures, we measure dipolar-like polarization patterns of the thermal radiation with high extinction ratios. Associated with these high extinction ratios for narrow and long heater structures, a significant enhancement of the thermal emission is observed. Our findings suggest the possibility of a strong infra-red near-field in the close vicinity of the nanoheaters with potential applications e.g. in microscopy.

3:42PM S44.00007 Plasmon Assisted Heating of Metal Nanoparticles. ADAM BUSHMAKER, University of Southern California, DAVID BOYD, California Institute of Technology, RAJAY KUMAR, University of Southern California, DAVID GOODWIN, California Institute of Technology, STEPHEN CRONIN, University of Southern California — Optical heating of Au nanoparticles by light at the plasmonically resonant frequency is studied. Block copolymer lithography is used to create highly uniform monodisperse arrays of Au nanoparticles. Extremely high temperatures and electric fields are produced locally with relatively low intensities of laser light. The heating is quantified using three approaches: melting of glass, dissociation of carbon monoxide, and Stokes/anti-Stokes Raman spectroscopy. Temperatures in excess of 370°C are observed in the nanoparticles. By focusing light into gaps of less than 70x10^3 W/cm^2. Anti-Stokes/Stokes Raman spectra of PbO deposited by plasmon assisted chemical vapor deposition (PACVD) [1] on top of the nanoparticles show a heating factor 1570 times larger than a bulk reference sample. We show that temperature rises of this magnitude are consistent with our model of reduced heating at the nanoscale. [1] D. A. Boyd et al, Nano Lett., 6, 2592 (2006).
3:54PM S44.00008 Modifying the visual appearance of metal nanoparticle composites by infrared laser annealing. ANDREJ HALABICA, Vanderbilt University, J. C. IDROBO, R. H. MAGRUDER III, R. F. HAGLUND JR., J. M. EPP, S. RASHKEEV, L. A. BOATNER, S. J. PENNYCOOK, S. T. PANTELIDES — It has long been known that noble-metal nanoparticles in insulators can alter their visual appearance. Many metal nanoparticle composites can be created by ion implantation and subsequent annealing to initiate phase separation, nucleation, and growth of nanoparticles. The size and size distribution of the nanoparticles and therefore the color of the composite are determined by the chemistry and thermodynamics of the annealing process. In this paper we report that we can also alter the color of gold- and silver-implanted silica and alumina by tunable infrared laser irradiation. Essentially a variant of rapid thermal annealing, this laser treatment can shift the plasmon band of the nanoparticles by tens of nm, resulting in significantly altered visual appearance. The amount of energy delivered to the implanted layer, and the subsequent color variation, can be adjusted by changing the wavelength and fluence of the laser. This makes it possible, as we will show, to write or pattern the composite material with 200 μm linewidths. This work is partially supported by DOE (DE-AC05-00OR22725), NSF (DME-0513048), and by Alcoa Inc.

4:06PM S44.00009 First Principles Absorption Spectra of Siₖ (n = 20 – 28) Clusters: TDLDA versus Predictions from Mie Theory. KOBBLAR JACKSON, Central Michigan University, JUAN C. IDROBO, SERDAR OGUT, University of Illinois at Chicago, MINGLI YANG. Central Michigan University — First-principles absorption spectra calculated within the time-dependent local-density approximation for Siₖ (n = 20 – 28) clusters reveal that prolate and compact clusters have distinct shape signatures, but no clear size dependence for a given shape. The size dependence and size index of the spectra and most of the peak positions and intensities can be explained remarkably well within the classical Mie theory, developed for light absorption by metallic particles using the bulk dielectric function of Si. Moreover, the experimental spectrum of Si₁₂ is in very good agreement with the theoretical spectrum of the prolate cluster, which is lower in energy than the compact one at this size.

1Supported by DOE Grant Nos. FG02-03ER15488 and FG02-03ER15489

4:18PM S44.00010 Optical Properties of Cage Versus Space-Filling Gold Clusters: A TDLDA Study, WERONIKA WALKOSZ, JUAN C. IDROBO, SERDAR OGUT, University of Illinois at Chicago, JINLAN WANG, JULIUS JELLINEK, Chemistry Division, Argonne National Laboratory — Recent DFT computations have revealed that medium size Auₙ clusters form hollow cage and space-filling structures that are energetically competitive. In fact, for n = 32 and 50 the cage structures are more stable than their space-filling counterparts. Here we report results of large-scale computations on the optical absorption spectra of the most stable cage and space-filling forms of Auₙ, n = 32, 38, 44, 50. The computations are performed using the time-dependent linear-response functional formalism within the local-density approximation (TDLDA). We examine the trends in the low-energy (< 6 eV) parts of the spectra as a function of the cluster size and structure and compare them with the predictions of the classical Mie theory.

2Supported by DOE Grant No. DE-FG02-03ER15488

4:30PM S44.00011 Isomeric Forms, Polarizabilities, and Optical Absorption Spectra of Ag₁₁, SERDAR OGUT, JUAN C. IDROBO, University of Illinois at Chicago, KAROLY NEMETH, JULIUS JELLINEK, Chemistry Division, Argonne National Laboratory — First principles based computational results on the atomic structures, static polarizabilities, and optical absorption spectra of eight low-energy isomers of Ag₁₁ are presented and discussed. The computations were performed using the static and time-dependent formalisms of the density functional theory. Comparison of the computed spectra with those measured for Ag₁₁ embedded in Ar and Ne matrices shows that it is the spectrum of the lowest energy isomer that exhibits the best overall agreement with the experiment. The theoretical analysis indicates that the d electrons play a more important role in optical transitions in Ag₁₁ than in smaller Agₙ, n ≤ 8, clusters.

3Supported by DOE Grant No. DE-FG02-03ER15488

4:42PM S44.00012 Preparation and control of optical properties of plasmonic crystals using colloidal crystals as templates. ZHEN-LIN WANG, PENG ZHAN, NAI-BEN MING, National Laboratory of Solid State Microstructures, Nanjing University — Plasmonic crystals show promise for applications from optical, electronic devices, nanolithography, metamaterials to enhanced Raman scattering sensors. For such applications it is important to develop simple routes to prepare such metallic films with two-dimensional (2D) regular nanoscale ordering. We will show that templating against 2D colloidal crystal is a convenient route to prepare such crystals that are composed of rigid array of metal nanoparticles. We also discuss how to excise rational methods which allow control over the morphology of the crystal unit, thus tuning optical properties of the prepared plasmonic crystals. By implementation of physical, chemical or electrochemical deposition of metal in combination with micromolding, a variety of morphologies of the metallic nanoparticles can be created. The nanoscale morphology and optical transmission properties of the prepared 2D metallic membranes have been characterized.

1The National Natural Science Foundation of China and the State Key Program for Basic Research of China support this work.

4:54PM S44.00013 Optical Metamaterials at Near IR Range Fabricated by Nanoimprint Lithography. E. KIM, UC Berkeley, W. WU, E. PONIZOVSKAYA, HP Labs, Y. R. SHEN, UC Berkeley, A. BRATKOVSKY, S. Y. WANG, HP Labs, UC BERKELEY TEAM, HP LABS TEAM — Metamaterials operating at near-IR frequencies have been designed, fabricated by nanoscale imprint lithography (NIL), and characterized by laser spectroscopic ellipsometry. The structure was a metal/dielectric/metal stack "fishnet" structure that demonstrated negative permittivity and permeability in the same frequency region and hence exhibited a negative refractive index at a wavelength near 1.7 micron. The results of the transmittance and the reflectance measurements of the "fishnet" structure show a strong resonance appears in the vicinity of 1.67 micron. This resonance comes from the negative permittivity combined with the magnetic resonance. The position of the resonance agrees with predictions from FDTD simulation. This work demonstrates the feasibility of designing various optical negative-index metamaterials and fabricating them using the NIL as a low-cost, high-throughput fabrication approach.
5:06PM S44.00014 Nanoparticles in alumina: Microscopy and Theory, JUAN C. IDROBO, ANDREJ HALABICA, Vanderbilt University. SERGEY RASHKEEV, Center for Advanced Modeling and Simulation, Idaho National Laboratory. MICHAEL V. GLAZOFF, Alcoa Inc., LYNN A. BOATNER, Materials Science and Technology Division, Oak Ridge National Laboratory, RICHARD F. HAGLUND, Vanderbilt University, STEPHEN J. PENNYCOOK, Materials Science and Technology Division, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University — Transition-metal nanoparticles formed by ion implantation in alumina can be used to modify the optical properties of naturally oxidized and anodized aluminum. Here, we report atomic-resolution Z-contrast images using a scanning transmission electron microscope (STEM) of CoFe and other metal nanoparticles in alumina. We also report electron energy loss spectra (EELS) and relate them to visual appearance and optical properties. Finally, we report first-principles density-functional calculations of nucleation mechanisms for these nanoparticles. This research was sponsored by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, by NSF grant No. DMR-0513048, and by Alcoa Inc.

5:18PM S44.00015 Probing the Surface Guided Modes from Infrared to Ultraviolet by Fast Electrons, AYCAN YURTSEVER, MARTIN COUILLARD, DAVID A. MULLER, Cornell University — We use monochromated, 200 kV electrons with high spatial resolution to study guided modes and surface plasmons in thin silicon slabs. We observe, both theoretically and experimentally, the presence of multiple plasmonic modes in a range from infrared to ultraviolet. We observe one mode at a thickness of ~20 nm and up to five modes at a slab thickness of ~250 nm, which agrees remarkably well with the relativistic dielectric theory. Finally, we use our technique to examine effective dielectric medium theories by studying silicon nanoparticles embedded in silicon oxide, a materials system with potential technological applications.

Thursday, March 8, 2007 8:00AM - 11:00AM

Session U8 DMP: Focus Session: Superconductivity and Magnetism, Colorado Convention Center Korbel 1C

8:00AM U8.00001 Triplet superconductivity and the long-range proximity effect in superconductor/half-metallic ferromagnet systems, TEUN Klapwijk, TU Delft — No abstract available.

8:36AM U8.00002 Odd-frequency pairing in superconducting heterostructures, A.A. Golubov, University of Twente, The Netherlands, Y. TANAKA, T. YOKOYAMA, Nagoya University, Japan, Y. ASANO, Hokkaido University, Japan — We present a general theory of the proximity effect in junctions between unconventional superconductors and diffusive normal metals (DN) or ferromagnets (DF). We consider all possible symmetry classes in a superconductor allowed by the Pauli principle: even-frequency spin-singlet even-parity state, even-frequency spin-triplet odd-parity state, odd-frequency spin-triplet even-parity state and odd-frequency spin-singlet odd-parity state. For each of the above states, symmetry and spectral properties of the induced pair amplitude in the DN (DF) are determined. The cases of junctions with spin-singlet s- and d-wave superconductors and spin-triplet p-wave superconductors are addressed in detail. We discuss the interplay between the proximity effect and midgap Andreev bound states arising at interfaces in unconventional (d- or p-wave) junctions. The most striking property is the odd-frequency symmetry of the pairing amplitude induced in DN (DF) in contacts with p-wave superconductors. This leads to zero-energy singularity in the density of states and to anomalous screening of an external magnetic field. Peculiarities of Josephson effect in d- or p-wave junctions are discussed. Experiments are suggested to detect an order parameter symmetry using heterostructures with unconventional superconductors.

8:48AM U8.00003 Phase Diagram and Thermodynamic Properties of Layered Ferromagnet-Superconductor Nanostructures, PAUL H. BARSIC, ORIOL T. VALLS, University of Minnesota — We present results obtained by exact, fully self-consistent numerical solution of the microscopic Bogoliubov-DeGennes equations for Superconductor/Ferromagnet (S/F) nanostructures in the clean limit. We discuss the thermodynamics of SFS trilayers, including the complete phase diagram over experimentally relevant parameter range. Both the first order 0 to π transition and the second order transition to the normal state at Tc are included. We find excellent agreement between theoretical and experimental results for Tc. Other relevant quantities such as DOS, magnetization, and conductivity will also be discussed.

9:00AM U8.00004 Transition Temperature Shifts in Asymmetric FSF Multilayers, PAUL CADDEN-ZIMANSKY, Northwestern University, J. SAMUEL JIANG, JOHN PEARSON, Argonne National Laboratory, YAROSLAW BAZALIY, IBM Almaden Research Center, SAM BADER, Argonne National Laboratory — Ferromagnet-Superconductor-Ferromagnet multilayers, where the superconductor thickness is on the order of the coherence length, exhibit shifts in the superconducting Tc when the relative magnetization of the ferromagnetic layers is changed. However, experimental work has produced shifts orders of magnitude smaller than theoretically predicted. We investigate this discrepancy by examining multilayers where the thickness of the two ferromagnetic layers is varied. Our work indicates that differences between the superconductor-ferromagnet interfaces may play a role in explaining the discrepancy, and demonstrates how the use of hard vs. soft ferromagnets can effect these devices.

9:12AM U8.00005 Conductance spectra of ferromagnetic superconductors, JACOB LINDER, MARTIN GRONSLETH, ASLE SUDBO, Norwegian University of Science and Technology — Recent findings of superconductors that simultaneously exhibit multiple spontaneously broken symmetries, such as ferromagnetic order or lack of an inversion center and even combinations of such broken symmetries, have led to much theoretical and experimental research. Ferromagnetic superconductors represent a marriage of two physical phenomena that conventionally have been considered virtually incompatible. We here study quantum transport in a junction consisting of a ferromagnetic metal and a non-unitary p-wave ferromagnetic superconductor. Considering several different possible pairing symmetries, our results show how the magnitude of the superconducting gaps may be inferred from the conductance spectra, in addition to their relative orientation in momentum-space. Also, we investigate how the strength of the magnetic exchange energies on both sides of the junction affect these spectra.

1Supported by DOE, Office of Science, under contract No. DE-AC02-06CH11357

1Work supported by the Norwegian Research Council.
9:24AM U8.00006 Derivation of the Ginzburg-Landau equations of a ferromagnetic $p$-wave superconductor$^1$. ESKIL DAHL, ASLE SUDBO, Norwegian University of Science and Technology — We derive a Ginzburg-Landau free energy for a $p$-wave ferromagnetic superconductor. The starting point is a microscopic Hamiltonian including a spin generalised BCS term and a Heisenberg exchange term. We find that coexistence of magnetisation and superconductivity depends on the sign of the energy-gradient of the DOS at Fermi level. We also compute the tunnelling contribution to the Ginzburg-Landau free energy, and find expressions for the spin-currents and Josephson currents across a tunnelling junction separating two ferromagnetic $p$-wave superconductors.

$^1$Work supported by the Norwegian Research Council.

9:36AM U8.00007 Nearly ferromagnetic superconductors$^1$. DIETRICH BELITZ, QI LI, University of Oregon, TED KIRKPATRICK, University of Maryland — The coexistence of ferromagnetism and superconductivity has received substantial attention over the years$^1$. Here we report on a theory for the electromagnetic properties of superconductors in the paramagnetic phase near a ferromagnetic instability$^2$. Using a generalized Ginzburg-Landau theory, we have found that the magnetic flux expulsion capability of the superconductor gets stronger as the normal-state magnetic susceptibility increases. The temperature dependencies of the London penetration depth, the critical fields, and the critical current are all strongly affected by ferromagnetic fluctuations. For the critical current we find a temperature exponent $\alpha \approx 2$ over an appreciable temperature range. The extent to which proximity to magnetic criticality may be a viable explanation for recent observations in MgCuNi microfibres, which find $\alpha \approx 2$$^3$, is discussed.


9:48AM U8.00008 Anisotropic Pauli depairing effects and field-induced nodal excitations in superconductors without inversion symmetry. SATOSHI FUJIMOTO, Department of Physics, Kyoto University — Superconductors without inversion symmetry have been currently attracting much interest. Here, we investigate theoretically a novel effect in the vortex state realized when the magnitude of the spin-orbit splitting due to the inversion symmetry breaking (ISB) is of the same order as the superconducting gap. Such a situation with the small ISB may be relevant to a superconductor without inversion symmetry $Y_2C_3$, which was recently discovered by Akimitsu et al. We show that in this case the Pauli depairing effect is anisotropic in the momentum space, and thus induces nodal excitations even for s-wave superconductors. We calculate the density of states and the specific heat coefficient on the basis of the Eliashberg’s quasiclassical method, and compare the results with experiments for $Y_2C_3$.

10:00AM U8.00009 Superconducting properties and the Fermi surface in noncentrosymmetric CeRhSi$_3$. T. TERASHIMA, T. YAMAGUCHI, T. MATSUMOTO, S. UJI, National Institute for Materials Science, N. KIMURA, T. KOMATSUZAR, H. AOKI, Tohoku University, H. HARIMA, Kobe University — CeRhSi$_3$ is a recently-discovered noncentrosymmetric superconductor [Kimura et al., PRL 95, 247004 (2005)]. At ambient pressure, P, it orders antiferromagnetically below $T_N = 1.6$ K. $T_N$ decreases with $P$ above $\sim$8 kbar, and disappears somewhere above 20 kbar. Superconductivity is observed above $\sim$12 kbar. We have performed measurements of ac susceptibility and the de Haas-van Alphen effect (dHvA) with the field in the $c$ direction up to $P$ = 29.5 kbar. Remarkably high upper critical fields $B_{c2}$ are observed: e.g., $B_{c2}$ = 17.5 T at 0.46 K for $P$ = 29.5 kbar, where the superconducting transition temperature is only 1.1 K. The Fermi surface continuously evolves from $P$ = 0 to 29.5 kbar, and the effective masses decrease with $P$. We argue that these are consistent with theoretical scenarios ascribing antiferromagnetism to spin-density-wave formation. Analyses of dHvA oscillations in the mixed state seem to suggest an anisotropic superconducting energy gap.

10:12AM U8.00010 Surface states in non-centrosymmetric superconductors. ANTON VORONTSOV, ILYA VEKHTER, Louisiana state university — Since the discovery of superconductivity in $\text{CePt}_3\text{Si}$, there is a strong interest in superconducting materials without center of inversion. Lack of inversion symmetry results in strong spin-orbit interactions that lift the spin degeneracy and leads to the mixing of 'singlet' and 'triplet' pairing channels. We consider surface bound states of a superconductor with bulk spin-orbit interactions described by a Rashba term, $\alpha \cdot \mathbf{k}$. We find that the scattering of the quasiparticle off the interface strongly mixes the two bands of opposite helicity. We analyze the properties of the surface states that appear for different surface orientations, investigate their spin structure and their possible signatures in tunneling experiments.

10:24AM U8.00011 Magnetic penetration depth in noncentrosymmetric $\text{Re}_3\text{W}$. YURI ZUEV, Oak Ridge Nat’l Lab, VALENTINA KUZNETSOVA, JAMES THOMPSON, University of Tennessee, DAVID CHRISTEN, Oak Ridge National Lab — The magnetic penetration depth is one of the most fundamental characteristics of a superconductor. We report measurements of temperature dependence of the penetration depth $\lambda$ in $\text{Re}_3\text{W}$ — a superconductor without inversion symmetry. The penetration depth was extracted from dc magnetic susceptibility measured on aligned quenched powder in epoxy using a SQUID magnetometer. At present, based on the low-temperature behavior of the superfluid density $1/\lambda^2$, we see no evidence of unconventional behavior, i.e. we see a fully-gapped state. Higher resolution data at low temperatures are needed to decide the case. ORNL is managed by UT-Battelle, LLC for USDOE under contract DE-AC05-00OR22725.

10:36AM U8.00012 Helical and stripe vortex phases in non-centrosymmetric superconductors. ZHICHAO ZHENG, DANIEL AGTERBERG, RAMINDER KAUR, University Of Wisconsin-Milwaukee — When magnetic fields are applied to non-centrosymmetric superconductors, helical or stripe vortex phases are formed. We develop a quasiclassical microscopic theory for these phases. We will study the resulting phase diagrams and physical properties of these phases as a function of the relative density of states of the two spin-split bands and with varying Zeeman-field strength. We apply these results to $\text{CePt}_3\text{Si}$, $\text{CeRhSi}_3$, $\text{CeIrSi}_3$, $\text{KOs}_2\text{O}_6$, $\text{Li}_2\text{Pt}_3\text{B}$ and $\text{Li}_2\text{Pd}_3\text{B}$.

10:48AM U8.00013 Superconducting properties of noncentrosymmetric $\text{Mg}_{60}\text{Ir}_{19}\text{B}_{16}$. TOMASZ KLIMCZUK, Faculty of Applied Physics, Gdansk University of Technology, Poland and Condensed Matter and Thermal Physics, Los Alamos National Laboratory, USA, ROBERT J. CAVA, Department of Chemistry, Princeton University, Princeton NJ 08544, USA, JOE D. THOMPSON, Condensed Matter and Thermal Physics, Los Alamos National Laboratory, USA — The magnetic, electrical transport and specific heat properties of the new ternary boride superconductor $\text{Mg}_{60}\text{Ir}_{19}\text{B}_{16}$ ($T_C = 5K$) have been investigated. The polycrystalline $\text{Mg}_{60}\text{Ir}_{19}\text{B}_{16}$ sample was synthesized by reaction of Mg and Ir metal powders with amorphous boron powder. The material has a noncentrosymmetric crystal structure (I-43m) and therefore the superconducting properties are a subject of great interest.

$^1$Work was performed under the auspices of the US Department of Energy, Office of Science.
8:00AM U9.00001 Closing the Quantum Metrological Triangle, M. PAALANEN, Helsinki Univ Technol, Low Temp Lab, Espoo, Finland, A. KEMPPIKENG, A. MANNINEN, A. SATRAPINSKI, MIKES, Espoo, Finland, J. HASSEL, P. HELISTO, A.O. NISKANEN, HEIKKI SEPPA, VTT Informat Technol, Espoo, Finland, P. HAKONEN, MIKKO MOTTONEN, JUKKA PEKOLA, JUHA VARTIAINEN, Helsinki Univ Technol, Low Temp Lab, Espoo, Finland — Quantum Metrological Triangle is made out of Josephson voltage standard, Quantum Hall resistance standard and an accurate current pump. Closing the Triangle consists of applying Ohm’s law with great accuracy on the three devices, based on fundamental physical phenomena and quantities, such as Planck’s constant and electron charge. The first two devices are already accepted international metrological standards. Recently we have made progress in developing the missing components for the closing experiments, i.e. a differential low-noise amplifier for comparing small currents and an accurate current pump. Both of these new devices are based on superconducting single electronics. We will describe our plans for closing the Triangle along with the expected uncertainties and also report on the progress in developing the low noise current amplifier and the current pump.


8:24AM U9.00003 Optimization of sensing coil geometry for low-field SQUID MRI and MEG.

8:36AM U9.00004 Noise Temperature of the Microstrip SQUID Amplifier with Cooling Fins.

9:00AM U9.00006 Symmetry of Charge and Thermal Transport in Andreev Interferometers.

9:12AM U9.00007 Few quasiparticle dynamics with a single-Cooper-pair transistor.
9:24AM U9.00008 High Frequency Flux Sampling SQUID Microscope\(^1\) , C.P. VLHACOS, Laboratory for Physical Sciences and University of Maryland, J. MATTHEWS, S.P. KWON, F.C. WELSTOOG, University of Maryland — One important application of scanning SQUID microscopes is to fault detection in integrated circuits and multi-chip modules. However, the present generation of computer processors operate at over 1 GHz, well above the bandwidth of the present generation of SQUID microscopes. We have overcome the bandwidth limitations of traditional scanning SQUID microscopes by removing the main bandwidth limiter – the conventional flux-locked loop electronics – and using instead a pulsed sampling technique with a hysteretic dc SQUID. We present time-varying magnetic field images obtained with the 4.2 K cryocooled microscope with a time-resolution below 1 nanosecond, and discuss the advantages and limitations of this method.

\(^1\)Supported by CSR, Neocera, Inc. and LPS.

9:36AM U9.00009 Fast NDE of Superconducting Magnet Wires using a Flow-Through SQUID Microscope with Coaxial Current Injection\(^1\) , J. MATTHEWS, F.C. WELSTOOG, University of Maryland, H. WEINSTOCK, Air Force Office of Scientific Research — We have developed a cryocooled high-Tc SQUID microscope for fast non-destructive evaluation (NDE) of long wires, designed for detecting defects in superconducting magnet wire. A feedthrough mechanism pulls the wire at speeds of up to 20 cm/s through a thin mylar tube that separates the room temperature wire from the SQUID. In order to null the magnetic field from bulk current flow the current return path is coaxial with the wire. We present results on test wires and samples of NbTi superconducting wire. By comparison with analytical and numerical models, we extract information from the data, such as defect size and location, and also outline a method for fast automated detection of defects in long wires.

\(^1\)Supported by AFOSR and the Center for Superconductivity Research.

9:48AM U9.00010 A three-junction single electron transistor as a diffusive, high-speed thermometer: Experiment and simulation , LOREN SWENSEN, D.K. WOOD, A.N. CLELAND, University of California, Santa Barbara, PHYSICS TEAM — Nanoscale calorimetry promises unprecedented sensitivity and temporal resolution for energy measurements in mesoscopic systems. As the size scale and temperature of a calorimeter are reduced, the heat capacity and equilibration time decrease rapidly. Achieving the lowest temperatures at the smallest size scales therefore requires thermometric sensors that can be operated with large measurement bandwidths (>1 MHz), at low temperatures (<1 K), and that minimally perturb the calorimeter itself. We have fabricated a unique, three junction single-electron transistor that allows diffusive thermometric sensing of a nanoscale calorimeter, with minimal power dissipation in the calorimeter volume. In this talk, we will describe the experiment, and our development of a Monte Carlo method to simulate the experimental device. Design optimization, sensitivity and practical implementation considerations will be discussed.

10:00AM U9.00011 Ultra-Sensitive Hot-Electron Detectors of IR/sub-mm Radiation , WEI JIAN, DAVID OLAYA, SERGEY PEREVERZEV, MICHAEL GERSHENSON, Rutgers University, BORIS KARASIK, JPL, Caltech, ANDREW SERGEEV, SUNY at Buffalo — We have developed a superconducting nanostructure that enables an ultra-sensitive detection of far infrared (FIR) and sub-mm radiation. The nanostructure consists of a Ti nanobridge with a volume of \(3 \times 10^{-13} \, \mu m^3\) flanked with Nb current leads. The electrons in the nanostructure are thermally isolated from the heat bath due to Andreev reflection from superconducting Nb leads and a weak electron-phonon coupling at mK temperatures. Being driven into the resistive state by the temperature and/or magnetic field, this transition-edge sensor is very sensitive to electron overheating. According to our measurements of the thermal conductance between the electrons in the nanobridge and the heat bath, the expected noise equivalent power and the response time of the detector at \(T=0.1 \, K\) are \(\sim 10^{-20} \, W/Hz^{1/2}\) and \(\sim 1 \, ms\), respectively. Alternatively, this nanostructure with a heat capacity \(C \sim 10^{-19} J/K\) at \(T=0.1 \, K\) can be used for the calorimetry of photons and phonons with an energy resolution \(\sim 10^{-21} J\). This resolution is sufficiently high for the detector to operate in a regime of THz photon counting.

10:12AM U9.00012 Microwave Techniques for SQUID Multiplexing , JOHN MATES\(^2\), University of Colorado, KENT IRWIN\(^3\), LEILA VALE\(^3\), GENE HILTON\(^4\), KONRAD LEHNERT\(^5\), MANUEL CASTELLANOS-BELTRAN\(^6\), NIST TEAM, JILA TEAM, UNIVERSITY OF COLORADO TEAM — A single Superconducting Quantum Interference Device, or SQUID, is a particularly good low-noise, low impedance amplifier. However, many applications for which SQUID’s are well-suited, ranging from astronomical spectroscopy to nuclear non-proliferation verification, require a large array of amplifiers. Large arrays require multiplexing techniques. Our group at NIST has developed several multiplexed SQUID arrays, including 1,280 pixel array of amplifiers. Large arrays require multiplexing techniques. Our group at NIST has fabricated several multiplexed SQUID arrays, including 1,280 pixel arrays, that use a time-division multiplexing technique. I will present work on existing SQUID multiplexing techniques and the development of a SQUID multiplexer operating at microwave frequencies. This new technique uses non-hysteric, non-dissipative rf-SQUID’s to tune microwave resonators, so that, with high enough Q’s, potentially tens of thousands of SQUID’s could be read out on one coaxial line. I will also report on our initial experimental work, in which we have demonstrated Q’s of around 100,000.

\(^2\)John Arthur Benson Mates \(\dagger\)-full name

\(^3\)NIST

\(^4\)NIST

\(^5\)JILA-University of Colorado

\(^6\)JILA-University of Colorado

10:24AM U9.00013 Superconducting Tunnel Junctions as Submillimeter Direct Detectors , JOHN TEUFEL, Yale University, MINGHAO SHEN, Yale University, LUIGI FRUNZIO, Yale University, DANIEL PROBER, Yale University, ROBERT SCHOELKOPF, Yale University, DEPTS. OF PHYSICS AND APPLIED PHYSICS COLLABORATION — We are developing superconducting tunnel junctions (STJ) as direct detectors for submillimeter astronomy. Photons with energy greater than the superconducting gap of the aluminum absorber break Cooper pairs and generate excess quasiparticles that are then measured as a tunneling current through the STJ. In order to monitor the response of the detector with large readout bandwidth and maximal sensitivity, we have implemented a novel readout which monitors the impedance of the detector via radio frequency (RF) reflectometry. For calibration of the detector, we have also developed a gold microbridge as an on-chip, submillimeter photon source. When biased, high frequency noise from the microbridge couples via a transmission line to the detector. This allows for a calibrated photon source with near unity coupling, fast chopping, and calibrable resolution. We will present results in the form of noise and responsivity properties of the STJ using the microbridge source and RF-STJ readout at 300 mK, demonstrating good responsivity, high sensitivity, and fast response times.
We have recently evidenced high Curie temperature ($T_C$) in self-assembled GeMn nanocolumns. From Transmission Electron Microscopy (TEM) cross sections we could clearly evidence that nano-columns are crossing the whole GeMn film. SQUID measurements reveal a high Curie temperature ($>400$ K) and Zero Field Cooled-Field Cooled (ZFC-FC) data rule out the presence of superparamagnetic nanoparticles. Growth is performed by simultaneously evaporating Ge and Mn atoms from standard effusion cells on Ge(001) single crystal substrates. The growth temperature is varied from 80 to 200 °C. In the whole temperature range, Mn-rich nano-columns are clearly observed by TEM. However magnetic properties depend on the growth temperature and high $T_C$-columns are only obtained in a very narrow temperature range around 130 °C. Magnetotransport measurements were performed with magnetic fields applied perpendicular to the film plane. A large positive magnetoresistance (up to 7000 % at 30 K) in contradiction with the negative MR in granular systems or other ferromagnetic semiconductors is measured. Taking MR effects into account we have evidenced a large Anomalous Hall Effect (AHE) up to room temperature despite of the low volume fraction of nano-columns in GeMn films. The presence of AHE proves that holes are spin-polarized by crossing nano-columns. In this presentation, we will discuss the kinetic mechanisms leading to the columns formation, the composition and crystal structure of the columns as well as their magnetic properties as a function of the growth temperature and Mn concentration.

This research has been supported by the Army Research Office.

10:36AM U9.00014 Single Crystal Superconducting Bolometric Photon Detector. KEVIN INDERHEE, PAUL WELANDER, JAMES ECKSTEIN, Department of Physics and F Seitz Materials Research Laboratory, University of Illinois, Urbana — We have studied bolometric photon detectors made from 10 nm thick single crystal niobium films grown by MBE. The films are atomically flat, have transition temperatures above 7.5 K and residual resistivity ratios $> 10$, and can be patterned with uniform cross section, since they are not granular. The critical current density at 4.2 K is greater than $2 \times 10^7$ A/cm$^2$. The films are patterned into links between 300 and 500 nm wide. As a function of bias current, the detectivity is sharply peaked near the critical current, which appears to increase the sensitivity. The detected voltage signal has been studied at low frequency so far ($\sim 1$MHz), and is linearly dependent on the photon flux. The fact that relatively wide links provide good detectivity is due to the uniform superconducting transport properties of the single crystal niobium.

Thursday, March 8, 2007 8:00AM - 11:00AM — Session U12 GMAG DMP FIAP: Focus Session: Diluted Magnetic Semiconductors II Colorado Convention Center Korbel 3C

8:00AM U12.00001 High Curie temperature ferromagnetism in self-organized GeMn nanocolumns. MATTHIEU JAMET, CEA-Grenoble, France — We have recently evidenced high Curie temperature ($T_C > 400$ K) Mn-rich nanocolumns self-assembled in a diluted Ge$_{0.94}$Mn$_{0.06}$ film. Their composition is close to Ge$_2$Mn as given by nanoscale chemical analysis (Electron Energy Loss Spectroscopy). Their average diameter, height and spacing are 3 nm, 80 nm and 10 nm respectively. Their volume fraction in the GeMn film is almost 16 %. From Transmission Electron Microscopy (TEM) cross sections we could clearly evidence that nano-columns are crossing the whole GeMn film. SQUID measurements reveal a high Curie temperature ($> 400$ K) and Zero Field Cooled-Field Cooled (ZFC-FC) data rule out the presence of superparamagnetic nanoparticles. Growth is performed by simultaneously evaporating Ge and Mn atoms from standard effusion cells on Ge(001) single crystal substrates. The growth temperature is varied from 80 to 200 °C. In the whole temperature range, Mn-rich nano-columns are clearly observed by TEM. However magnetic properties depend on the growth temperature and high $T_C$-columns are only obtain in a very narrow temperature range around 130 °C. Magnetotransport measurements have been performed with magnetic fields applied perpendicular to the film plane. A large positive magnetoresistance (up to 7000 % at 30 K) in contradiction with the negative MR in granular systems or other ferromagnetic semiconductors is measured. Taking MR effects into account we have evidenced a large Anomalous Hall Effect (AHE) up to room temperature despite of the low volume fraction of nano-columns in GeMn films. The presence of AHE proves that holes are spin-polarized by crossing nano-columns. In this presentation, we will discuss the kinetic mechanisms leading to the columns formation, the composition and crystal structure of the columns as well as their magnetic properties as a function of the growth temperature and Mn concentration.

8:36AM U12.00002 Dopant segregation and giant magnetoresistance in manganese-doped germanium. A.P. LI, Oak Ridge National Lab, C. ZENG, University of Tennessee, K. VAN BENTHEM, M.F. CHISHOLM, J. SHEN, Oak Ridge National Lab, S.V.S. NAGESWARA RAO, S.K. DIXIT, L.C. FELDMAN, Vanderbilt University, A.G. PETUKHOV, M. FOYLEG, South Dakota School of Mines and Technology, H.H. WEITERING, University of Tennessee — Dopant segregation in Mn$_{0.5}$Ge$_{1-x}$ dillute magnetic semiconductor lead to a remarkable self-assemble of Mn-rich nanocolumns, embedded in a fully compensated Ge matrix. Samples grown at 80 °C display a giant positive magnetoresistance that correlates directly with the distribution of magnetic impurities. Annealing at 200 °C increases substitution in the host matrix above the threshold for the insulator-metal transition, while maintaining the columnar morphology, and results in global ferromagnetism with conventional negative magnetoresistance. The qualitative features of magnetism and transport in this nanophase material are thus extremely sensitive to the precise location and distribution of the magnetic dopants.

8:48AM U12.00003 Ferromagnetism in Mn doped Ge thin films. JIANI YU, JIWEI LU, KEVIN WEST, LI HE, ROBERT HULL, STU WOLF, University of Virginia, MATERIAL SCIENCE AND ENGINEERING, UNIVERSITY OF VIRGINIA TEAM — Exploring ferromagnetism in Group IV semiconductors is of great interest due to their potential application to spintronics. In this presentation, we discuss the ferromagnetism induced in thin Ge films by Mn$^+$ ion implantation as well as the correlation between their magnetism and their transport properties. The as-received Germanium on Insulator (GOI) wafer consists of 200nm of (100) oriented Ge on 400nm of oxide both on a Si wafer. Mn ions were implanted at 300 °C into the Ge layer at 200 KeV. The ferromagnetism has been observed in Ge with a range of Mn concentration from 0.5 to 2 atom %. The sample with 2 % Mn doping has a Curie temperature near 300K and has a moment of $0.7 \mu_B$/Mn at 10 K. Transmission electron microscopy (TEM) reveals the formation of second phase clusters of which are probably responsible for the majority of the magnetism in this sample. In contrast, the 0.5 % and 1 % Mn as implanted Ge thin films behave like diluted ferromagnetic semiconductors, both have Curie temperatures is around 100 ~150 K and the 0.5% sample doesn’t show TEM evidence of a second phase. Our data indicates that the transport properties of Mn doped Ge correlates with the magnetism.

9:00AM U12.00004 Effects of complementary doping of transition metals into Ge epitaxial films. BRIAN COLLINS, LIANG HE, FRANK TSUI, University of North Carolina, YUNCHENG ZHONG, STEFAN VOGT, YONG CHU, Advanced Photon Source — We report structural and magnetic properties of epitaxial films of Co and Mn co-doped Ge, grown by combinatorial molecular beam epitaxy on Ge (001) substrates. A ternary epitaxial phase diagram has been determined for total doping concentrations up to 30 at. %, where regions of coherent epitaxy and associated strain states, and regions of rough disordered growth and the nature of the disorders have been examined and identified. In the phase diagram, there are two adjacent regions in composition, one Co-rich and another Mn-rich, where pseudomorphic epitaxial growth can be achieved at combined doping concentrations as high as 17 at. %. These values are significantly higher than those from using either of the dopants individually. The lattice constants of the Co-rich films obey the Vegard’s law, i.e. a linear dependence on the concentration, while the Mn-rich counterparts do not. This finding indicates that two transition metal dopants can compensate for the internal stress caused by the individual dopants in the host lattice. Our results also show that the presence of a second dopant can significantly reduce the tendency for phase separation and disorder, especially when Mn is the primary dopant. A ternary magnetic phase diagram has been determined using the magnetooptic Kerr effect, within which there exit high quality epitaxial films of magnetic semiconductors.
9:12AM U12.00005 Dopant-assisted Concentration Enhancement of Substitutional Mn in Si and Ge1. WENGUANG ZHU, Harvard University & The University of Texas at Austin & The University of Tennessee, ZHENYU ZHANG, ORNL & The University of Tennessee, EFTHIMIOS KAXIRAS, Harvard University — Incorporation of Mn atoms as magnetic impurities in bulk Si and Ge is of great importance for integrating magnetism with existing device technology. Here, we study the influence of p- and n-type electronic dopants on Mn incorporation in bulk Si and Ge, using first-principles calculations within density functional theory. We find that in bulk Si, the site preference of a single Mn atom is changed from interstitial to substitutional in the presence of a neighboring n-type dopant (P, As, Sb). In bulk Ge, a Mn atom is more easily incorporated into the lattice when an n-type dopant is present in its immediate neighborhood, forming a stable Mn/dopant dimer with both impurities at substitutional sites. A detailed analysis of magnetic exchange interactions between such dimers reveals that magnetic properties are not degraded when Mn atoms coexist with n-type dopants.

1Supported by NSF and DOE

9:24AM U12.00006 Interstitial Mn in Si: half-metallic heterostructures studied by density-functional theory. PETER KRATZER, University Duisburg-Essen, D-47048 Duisburg, Germany, HUA WU, University Cologne, D-50937 Cologne, Germany, MATTI MAASYRANTA, FI, MATTI KEMPPINEN, HANNES HUSKIALA, University of Helsinki, Finland, JURGEN HENNING, University Duisburg, Germany, ARI POITSINEN, University of Jyvaskyla, Finland, RAGHUVOORTHI SANTHOSH, University of Texas, Dallas, USA — Functional calculations that have been carried out to determine the strength of the distance-dependant exchange interaction in Mn-doped Si. The exchange interaction determines the energy difference between ferro-magnetic and anti-ferromagnetic spin configurations and as such it provides for a prediction of experimental achievement of above-room-temperature magnetism in Mn doped silicon (Phys.Rev.B 71, 033302 (2005)). We present the results of Density Functional calculations that have been carried out to determine the strength of the distance-dependant exchange interaction in Mn-doped Si. The exchange interaction determines the energy difference between ferro-magnetic and anti-ferromagnetic spin configurations and as such it provides for a prediction of spin-wave velocities. Such spin waves, if they exist, are of interest in that they may provide means for transmitting spin-based information. Comparison of the relative energy differences between ferromagnetic and anti-ferromagnetic configurations for a series of Mn locations yielded the distance dependent exchange interaction J(R). Interestingly we find that the exchange interaction is negative (anti-ferromagnetic) for short and long distances and is positive (ferromagnetic) for intermediate distances. This talk will present these findings along with estimates of spin-wave velocities, densities of states, band structure and spin-density distributions.

9:36AM U12.00007 Ge-Based Diluted Magnetic Semiconductor films on Si1. ZUOMING ZHAO, XIAOYU ZHOU, KANG L. WANG, University of California, Los Angeles — Ge-based diluted magnetic semiconductor (DMS) films with 4% Mn (MnGe) are grown on Si (001) substrates using molecular beam epitaxy (MBE). Surface morphology is measured by atomic force microscopy (AFM). For a 24-nm thick film, surface roughness around is around 1nm. Structure properties of the film are characterized by X-ray diffraction (XRD) and single crystal film quality by the results which only (004) Ge peak is observed. Magnetic properties are measured by a superconducting quantum interference device (SQUID). Clear hysteresis is observed at room-temperature. The results indicate that high quality Ge-based DMS can be grown on Si with good crystal quality and magnetic properties.

1MACRO Focus Center on Functional Engineered Nano Architectonics, Western Institution of Nanoelectronics

9:48AM U12.00008 Local moment and interaction of manganous moment in amorphous silicon thin films. LIZENG, University of California, San Diego, FRANCES HELLMAN, University of California, Berkeley, ROBERT CULBERTSON, RAFIQUIL ISLAM, DAVID SMITH, Arizona State University, ERIK HELGREN, University of California, Berkeley — Highly homogeneous Mn doped amorphous silicon (a-Mn_xSi_1−x) was prepared by direct MBE deposition. Magnetic exchange interaction between interstitial Mn and Si is, in its infancy. So far, research on Mn-doped Si has concentrated on substitutional Mn (Mn_sub) as done for Mn-doped GaAs and Ge, although Mn_sub impurities in Si are energetically less stable than interstitial Mn (Mn_int). In this work, we investigate the role of Mn_int impurities for ferromagnetism in Si, and propose a novel type of heterostructures with Mn_int δ-doping. Using density-functional theory within the generalized gradient approximation, we show that Si-based heterostructures with 1/4 layer δ-doping of Mn_int are half-metallic. For Mn_int concentrations of 1/2 or 1 layer, the δ-doped heterostructures still display a high spin-polarization of conduction electrons, about 85% and 60%, respectively. The proposed heterostructures are more stable than previously assumed δ-layers of Mn_sub. Contrary to wide-spread belief, the present study demonstrates that interstitial Mn can be utilized to tune the magnetic properties of Si, and thus provides a new clue for Si-based spintronics materials.

10:00AM U12.00009 Spin waves in Mn-doped Si: exchange interactions from first-principles calculations. G. RAO and J. E. Raynolds College of Nanoscale Science and Engineering, University at Albany, State University of New York, GAYATHRI RAO, JAMES RAYNOLDS, CNSE, University at Albany — There has been considerable interest in magnetic semiconductors in recent years for potential applications in the field of spintronics. The present work was motivated by recent experimental achievement of above-room-temperature magnetism in Mn doped silicon (Phys.Rev.B 71, 033302 (2005)). We present the results of Density Functional calculations that have been carried out to determine the strength of the distance-dependant exchange interaction in Mn-doped Si. The exchange interaction determines the energy difference between ferro-magnetic and anti-ferromagnetic spin configurations and as such it provides for a prediction of spin-wave velocities. Such spin waves, if they exist, are of interest in that they may provide means for transmitting spin-based information. Comparison of the relative energy differences between ferromagnetic and anti-ferromagnetic configurations for a series of Mn locations yielded the distance dependent exchange interaction J(R). Interestingly we find that the exchange interaction is negative (anti-ferromagnetic) for short and long distances and is positive (ferromagnetic) for intermediate distances. This talk will present these findings along with estimates of spin-wave velocities, densities of states, band structure and spin-density distributions.

10:12AM U12.00010 Controlling magnetic, magnetotransport and optical properties of Al codoped Zn-Co-O thin films. PLAMEN STAMENOV, CRANN and School of Physics, Trinity College, Dublin 2, M. VENKATESAN, L. DORNELES, J.M.D. COEY, MANSE TEAM — Thin films of 5% Co doped ZnO were grown on C- and R-cut sapphire substrates by pulsed-laser deposition, with and without Al doping (x=0–1% Al). Al-doped films retain significant magnetization while exhibiting degenerate semiconductor behaviour. Magnetoresistance of these novel Co-doped ZnO semiconductor films is found to be highly dependent on Al doping and is vanishingly small at (x>0.2 %) Large (~20 % at 2K) in-plane anisotropy of the magnetoresistance is observed, resembling an AMR effect, which is attributed to Fermi surface anisotropy and most of it has no “ferromagnetic” origin. The field dependence of the magnetoresistance can be explained in terms of two-band model and ionised impurity scattering. Hall-effect data indicates completely degenerate electron gas at (x=0.5 %). High resolution x-ray scattering and magnetisation data on samples with (x=0) reviles the presence of Co metal clusters (~8nm in size) that account for much or all the ferromagnetic magnetisation and exhibit temperature activated decrease of the coercive field. A huge band gap shift is observed with Al doping as a result of Burstein-Moss effect. In view of the vanishing magnetoresistive effects at room temperature, it is clear that these Co doped ZnO samples are not dilute magnetic semiconductors.
10:24AM U12.00011 Electrical transport and magnetic properties of sputtered Co-doped indium-tin oxide films. JOLANTA STANKIEWICZ, ICMA, CSIC-Universidad de Zaragoza, FRANCISCO VILLUENDAS, Departamento de Física Aplicada, Universidad de Zaragoza — We report results of electrical resistivity, Hall effect and magnetization measurements in Co-doped indium-tin oxide films, in a temperature range from 5 to 400 K and in magnetic fields of up to 5 T. The films were grown on fused quartz substrates, by magnetron sputtering. ITO (In_{2}O_{3} with 10 wt % Sn) homogeneous films doped with less than 20 at. % of Co seem to show intrinsic FM behavior. Magnetic hysteresis loops with coercive fields of up to 100 Oe at room temperature, as well as a ferromagnetic contribution in the difference between field-cooled and zero field-cooled magnetization, are observed in these films. We find that post-growth treatment strongly affects the electrical and magnetic properties of our films. This allows us to control the electron concentration of the films by varying the temperature and/or changing the ambient gas in the annealing process. A clear correlation between the values of the magnetic moment and of the electron concentration found for the ITO films doped with 10 at. % of Co seems to follow the predictions for a bound magnetic polaron percolation model. This suggests a carrier-mediated ferromagnetic mechanism.

10:36AM U12.00012 Investigation of Mn incorporation on GaN(0001) by spin-polarized STM. YUN QI MI, WEINERT, L. LI — We investigate the Mn substitution of Ga on GaN(0001) by spin-polarized scanning tunneling microscopy (SP-STM) using a Fe coated W tip. The GaN films are grown by plasma-assisted MBE on 6H-SiC(0001), with a metallic pseudo-1x1 denoted “1x1” surface, consists of 2.3 ML Ga on top of the Ga-terminated GaN. Mn deposition on this surface results in the formation of domains of 5x5 and 5√3 x 5√3 structures. First principles calculations show that Mn substitution of Ga leads to virtual bound states with bandwidth of ~1.5 eV, indicating significant Mn-Ga interactions. We propose that Mn substitution of Ga creates the Ga motion in the adlayer of the “1x1”, forcing the extra Ga atoms of the top layer to “pop-up” and reside at the T₃ sites, forming the (5x5) reconstruction similar to the DAS structure observed on Si(111) surface. With the Fe/W tip, the regions that contain the incorporated Mn would give rise to the extra bright features that form the 5√3 x 5√3 structure, due to the higher spin DOS at Mn sites. Implications of these results for understanding the magnetic coupling between Mn atoms in GaN will be discussed at the meeting.

1Supported by DOE (DE-FG02-05ER46228).

10:48AM U12.00013 Electrical manipulation of non-volatile spin cell based on diluted magnetic semiconductor quantum dots. KI WOOK KIM, North Carolina State University — Electrical manipulation of a memory cell based on a semiconductor nanostructure consisting of a diluted magnetic semiconductor quantum dot (QD) and a reservoir of itinerant holes separated by an energy barrier is investigated theoretically. The operating principle takes advantage of the paramagnetic-ferromagnetic phase transition mediated by the itinerant holes in the diluted magnetic semiconductor QD that can lead to electrically controlled Write/Erase operations. Non-volatility can be achieved when the structure is properly designed to reach a thermodynamic equilibrium at both the PM and FM configurations. Assuming a parabolic confining potential in the QD, the performance characteristics of the proposed nanostructure are analyzed including the scalability and the lifetime. An advantage of this memory concept is the extremely small dissipative energy for Write/Erase functions due to the open circuit nature of the process. A readout scheme enabling electrical detection with the repetition rate up to the 10 - 100 MHz range is also explored by utilizing only two contacts.

Thursday, March 8, 2007 8:00AM - 11:00AM — Session U13 DMP GMAG: Focus Session: Magnanites, Titanates, & Vanadates Colorado Convention Center Korbel 4C

8:00AM U13.00001 Combining DFT and Many-body Methods to Understand Correlated Materials. IGOR SOLOVYEV, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan — Electronic and magnetic properties of strongly-correlated systems are typically controlled by a limited number of electronic states, located near the Fermi level and well isolated from the rest of the spectrum. This opens a formal way for combining the first-principles methods of electronic structure calculations, based on the density-functional theory (DFT), with model many-body methods, formulated in a restricted Hilbert space of states near the Fermi level. The core of this project is the construction of “ab initio model Hamiltonians”, which would incorporate the physics of on-site Coulomb correlations and provide a transparent physical picture for the low-energy properties of strongly- correlated systems. First, I will describe a systematic procedure for constructing such an effective Hubbard-type model, which consists of three major steps, starting from the electronic structure in the local- density approximation. (i) Construction of the kinetic-energy part using an exact version of the downfolding method, (ii) Construction of the Wannier functions, (iii) Calculation of screened Coulomb interactions using a hybrid approach, which combines the random phase approximation with the constraint DFT. Then, I will illustrate abilities of this method for resolving a number of controversial issues, related with the interplay of the experimental lattice distortion and magnetic properties of four narrow t₂g band persovskite oxides (YTO₃, LaTiO₃, YVO₃, and LaVO₃), for which the obtained Hamiltonian was solved using a number of techniques, including the Hartree-Fock (HF) approximation, the second-order perturbation theory and the t₄ matrix approximation for the correlation energy, and a variational superexchange theory, which takes into account the multiplet structure of the atomic states. I will argue that the crystal distortion imposes a severe constraint on the form of the possible orbital states, which favors the formation of experimental magnetic structures in YTO₃, YVO₃, and LaVO₃, even at the level of HF approximation. The correlation effects systematically improve the agreement with the experimental data and additionally stabilize the experimentally observed G- and C-type antiferromagnetic states in YVO₃ and LaVO₃. The role of relativistic spin-orbit interaction will be also discussed.

8:36AM U13.00002 Additional evidence for complex 2-site polarons in CMR manganites. FRANK BRIDGES, GEZA KURCZVEIL, LISA DOWNWARD, UC Santa Cruz, JOHN J. NEUMEIER, Montana State University — Recently we have proposed a complex 2-site polaron model (which we call a dimer) that exists for temperatures near and above the ferromagnetic transition temperature, Tᵢ. The dimer has a hole delocalized over two Mn sites (i.e., one hole and an electron share the two Mn sites) and the two Mn sites have a reduced distortion compared to the remaining Jahn-Teller distorted electron sites. Magnetic clusters just above Tᵢ are likely clusters of these dimer quasiparticles. The average valence of the two Mn sites in the dimer is 3.5 and the spin is 7/2. We show that the Mn K-absorption edge is much better described as a sum of a 3.5 valence edge (fraction 2x) plus a 3 valence edge (fraction 1x), compared to earlier simulations using x CaMnO₂ plus y LaMnO₃. We also show that fitting the Mn-O peak to a sum of two experimental Mn-O standards leads to a similar result as in the earlier study — a fraction 2x of lower distorted Mn sites (dimers) and a fraction 1-2x of more distorted sites with 1 eₒ electron. Both support the proposed complex 2-site polaron model.

Supported under NSF grant DMR0301971.

1I. V. Solovyev, Z. V. Pchelkina, and V. I. Anisimov, cond-mat/0608528.
1I. V. Solovyev, cond-mat/0608625.

1Which to express my thanks to Masatoshi Imada for valuable interactions on the early stages of this project.

9:48AM U13.00003 Magnetic mapping of phase separated manganite films1. CASEY ISRAEL, DIANA SANCHEZ, TAKESHI KASAMA, RAFAEL DUNIN-BORKOWSKI, NEIL MATHUR, Department of Materials Science and Metallurgy, University of Cambridge, TIEN-MING CHUANG, ALEX DE LOZANNE, Physics Department, University of Texas at Austin — We summarize the recent results of efforts to image the different phases in phase-separated epitaxial thin manganite films. We present images acquired by three techniques, electron holography in a transmission electron microscope, magnetic force microscopy (MFM), and conducting atomic force microscopy (CAFM), all of which are applied to La1-xCaxMnO3 (LCMO) films grown on NdGaO3 (001) substrates. Electron holography images of a focused ion beam milled LCMO ($x = 0.3$) film (uniformly ferromagnetic at low temperatures) demonstrate the feasibility of using this method to distinguish local phases with different magnetic properties and illustrate the dangers of ion implantation during focused ion beam processing. MFM and CAFM scans of an as-deposited LCMO ($x = 0.40$) film (phase-separated at low temperatures) indicate the coexistence of ferromagnetic (metallic) and nonferromagnetic (insulating) regions characterized by length scales below roughly 100 nm. It appears that the ferromagnetic regions preferentially form conducting pathways aligned with the film’s easy-axis for magnetization. This seems intrinsic, in that there are no topographical features linked with this phase anisotropy.

1 Funded by the EU (STRP) and the NSF.

9:00AM U13.00004 Observation of Nanoscale Electronic Phase Separation and Charge Density Wave in Manganites. JEEHOON KIM, JINWEI HUANG, ALEX DE LOZANNE, Department of Physics, University of Texas at Austin, J. S. ZHOU, J. B. GOODENOUGH, Texas Materials Institute, University of Texas at Austin — Scanning tunneling microscopy (STM) is used to image the surface topography and local density of states (LDOS) in the bilayer colossal magnetoresistance (CMR) material LSMO below the Curie temperature. While our STM is capable of atomic resolution, on this surface the smallest features are randomly distributed islands with a lateral size of ~1 nm. We obtained conductance maps to investigate the local electronic structure associated with these islands. The 2-D cross-correlation map between the gap map and the topography suggests a random distribution of three different domains which are Mn3+ rich, Mn4+ rich or mixed valence Mn11/4. The spectroscopic data show a large gap around 600 meV. We also observed some modulations in the conductance map. The Fourier transform of the conductance map shows two major modulations with 1.6 nm and 60 nm wavelength along the crystal axis. The 1.6 nm wavelength modulation can be explained by charge density wave (CDW) model resulting from a Fermi surface instability.

9:12AM U13.00005 Susceptibility imaging of a weakly disordered manganite in high magnetic field. WEIDA WU, Dept. of Physics and Astronomy, Rutgers University, CASEY ISRAEL, Department of Materials Science and Metallurgy, University of Cambridge, ALEX DE LOZANNE, Physics Department, University of Texas at Austin, NAM JUNG HUR, Department of Physics, Inha University, SOONYONG PARK, SANG-WOOK CHEONG, Dept. of Physics and Astronomy, Rutgers University — We report variable temperature magnetic force microscopy (VT-MFM) studies of (La,Pr)xCa0.375MnO3 in a 1 T magnetic field with temperature ranging from 10 K to 250 K. In-situ resistance measurements confirmed the bulk phase transitions between paramagnetic, anti-ferromagnetic charge ordering and ferromagnetic (FM) phases. Above the FM transition (~80K), MFM images show μm-scale magnetic contrast which originates from the local susceptibility variations of the different phases1. By comparing the MFM images with polarized optical microscopy images taken at room temperature, it becomes apparent that the magnetic phase inhomogeneity observed at elevated temperature is linked to local strain variations at the surface of the sample. The high field susceptibility imaging technique could be extended to the study of other magnetic phase separated systems.


9:24AM U13.00006 Evidences for Metal-Insulator Phase Coexistence Below Tc in Self-doped Manganese Films. PENG GAO, TREVOR A. TYSON, MICHAEL DELEON, New Jersey Institute of Technology, CATHERINE DUBOURDIEU, LGMP-Minatec, France, ZHENXIAN LIU, Brookhaven National Laboratory — We present evidence for the existence of a significant insulating phase component more than 100 K below the magnetic ordering temperature in the self-doped system La0.8Ca0.2MnO3. Reflectivity measurements were made over the range 100 to 8000 cm-1. Using the Drude-Lorenz Model, we convert reflectivity spectra into optical conductivity spectra. The insulating phase was evident as sharp resonances corresponding to atomic vibrational modes which disappeared deep in the metallic phase at low temperature. A significant component of the insulating phase exists down to 200 K below Tc. Between 200 K and 150 K, the metallic phase becomes the dominant phase. Comparisons are made with the La0.7Ca0.3MnO3 samples measured under the same conditions.

9:36AM U13.00007 Phase-segregated Glass Formation Linked to Long-Range Strain using Resonant Ultrasound Spectroscopy. PETER SHARMA, RIKEN (The Institute of Physical and Chemical Research), S. EL-KHATIB, I. MIHUT, J. B. BETTS, A. MIGLIORI, National High Magnetic Field Laboratory, Los Alamos, S. KIM, S. GUHA, S-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University — We have observed a very large damping of ultrasonic waves in the magnetically/structurally/structurally phase segregated state of a CMR manganite that suddenly disappears upon the formation of a glassy state. A subtle stiffening of the shear modulus accompanies the putative glass transition. Our observations most explicitly link strain to the proposed formation of an unusual glass state composed of coexisting, macroscopic structural domains found in this material. These results may implicate strain as the determining factor in the formation of non-equilibrium mixed-phase states in other systems that display widely hysteretic first order magneto-structural transitions.

9:48AM U13.00008 Raman scattering studies of field- and temperature-dependent melting of charge order in La0.25Pr0.375Ca0.375MnO3 and La0.5Ca0.5MnO31. MINJUNG KIM, H. BARATH, S.L. COOPER, Dept. of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana–Champaign, M. RUBHAUSEN, Institut für Angewandte Physik, University of Hamburg, Germany. — The La0.25Pr0.375Ca0.375MnO3 system provides an interesting opportunity to study the effects of chemical disorder—introduced by replacing La3+ with Pr3+ having a smaller ionic radius—on the charge-ordered (CO) state and the complex field- and temperature-dependent phase behavior observed in the manganese perovskite La1−x, Ca2MnO3. We report field- and temperature-dependent Raman studies of La0.25Pr0.375Ca0.375MnO3 and La0.5Ca0.5MnO3, in which we are able to carefully study the effects of disorder on both field-induced melting of CO and on the field-induced evolution of novel structural and magnetic phases in the (La,Pr)Ca2MnO3 system. Among other results we will discuss, La0.25Pr0.375Ca0.375MnO3 exhibits a quantum melting transition from a CO state to a ferromagnetic metal phase at fields less than 7 T, which is a much lower value than that observed in La0.5Ca0.5MnO3 (~20T).

1 Work supported by the Dept. of Energy under grant No. DEFG02-91ER45439
10:00AM U13.00009 Optical study of Nd$_{0.5}$Sr$_{0.5}$MnO$_3$ thin films on SrTiO$_3$, SEUNG YUP JANG, M.W. KIM, K.W. KIM, T.W. NOH, ReCOE & FPRD, Department of Physics and Astronomy, Seoul National University, Korea, N. NAKAGAWA, H.Y. HWANG, Department of Advanced Materials Science, University of Tokyo, Japan — Doped rare earth manganites show interesting phase diagrams depending on strong coupling among spin, charge, and orbital degrees of freedom. Especially, Nd$_{0.5}$Sr$_{0.5}$MnO$_3$ (NSMO) undergoes two phase transitions of para-magnetic insulating state to ferro-magnetic metallic state (FMM) and FMM to charge/orbital ordered insulating state as temperature decreases. When NSMO is grown as a thin film on SrTiO$_3$(STO) (001), it has no phase transition. Recently, however, thin films grown on STO (110) substrates were found to retain the phase transitions of bulk NSMO. This implies that the charge/orbital state could be modulated by control lattice strain. We have investigated the optical conductivity spectra of NSMO epitaxial thin films grown on STO substrates. Optical spectra of NSMO grown on STO (110) show drastic change, depending on temperature and polarization. Based on the careful comparison between the films grown on differently oriented STO substrates, we demonstrate that the substrates strain can cause crucial effect on the ground state of NSMO to result in a novel insulating state which is rarely known.

10:12AM U13.00010 Phase diagram for Bi$_1$-xCa$_x$MnO$_3$ (x < 0.5), YUHAI QIN, TREVOR TYSON, New Jersey Institute of Technology, SANG-WOOK CHEONG, Rutgers University, XIAONONG XU, Nanjing University — The multiferroic Bi$_x$MnO$_3$ system, in which ferroelectric and ferromagnetic orders can coexist, has attracted much research work in the past years for its potential technological applications. For the more general system Bi$_1$-xCa$_x$MnO$_3$, the phase diagram for the Ca rich region (x > 0.4) has been established [1]. In order to understand the multiferroic behavior near the x=0 system, the hole-doped region (0<x<0.5) was investigated. We have completed the magnetic, transport, and structural phase diagram of Bi$_1$-xCa$_x$MnO$_3$, by performing detailed structural (XRD and XAFS), magnetization (ZFC/FC) and electrical measurements on Bi$_1$-xCa$_x$MnO$_3$ (0<x<0.5), showing the transformation form the highly distorted monoclinic phase to the orthorhombic phase. This work is supported by NSF DMR-0512196. [1] H. Woo, T. A. Tyson, M. Croft, S. W. Cheong, and J. C. Woicik, Physical Review B: Condensed Matter and Materials Physics 63, 134412/1 (2001).

10:24AM U13.00011 ABSTRACT WITHDRAWN

10:36AM U13.00012 Investigation of the local Mn-O distortions in the concentration-induced Metal/Insulator transition materials, La$_{1-x}$Ca$_x$MnO$_3$ (x= 0.16-0.22) using EXAFS, 1 YU JIANG, LISA DOWNSWARD, FRANK BRIDGES, Physics Dept., University of California, Santa Cruz, JOHN NEUMEIER, Physics Dept., Montana State University — The pseudo-cubic manganites La$_{1-x}$Ca$_x$MnO$_3$ (LCMO) are CMR (Colossal Magnetoresistance) materials for x between approximately 0.2 and 0.5. They have a temperature driven metal/Insulator (MI) transition at the ferromagnetic transition temperature $T_c$, which is caused by Jahn-Teller-like distortions which form around Mn sites as $T$ increases through $T_c$. Near x=0.2 the MI is driven by concentration. To investigate the concentration and temperature dependent local distortions for low doped powder samples (LCMO x = 16%, 18%, 20%, 22%), we carried out EXAFS (Extended X-ray Absorption Fine Structure) experiment at SSRL (Stanford Synchrotron Radiation Laboratory). The results of our preliminary analysis show the following: (1) a sharp, step increase in $\sigma^2$ near $T_c$, ($\sigma$ is the width of the Mn-O pair distribution function (PDF)), (2) the magnitude of the step decreases rapidly with decreasing x, (3) the value of $\sigma^2$ at low T is close to the value for zero-point motion for x = 0.22, but increases substantially for lower x, indicating that in the magnetized state a large J-T distortions remain at low T for low x. Also the magnetization at low T is small for lower x, indicating that not all of the sample is ferromagnetic.

1Supported under NSF grant DMR0301971

10:48AM U13.00013 Temperature- and field-dependent far-infrared studies of (La$_{0.4}$Pr$_{0.6}$)$_{0.67}$Ca$_{0.33}$MnO$_3$ films 1, NAVEEN MARGANKUNTE, TARA P. DHAKAL, Dept of Physics, Univ of Florida, ALEXANDRE ZIMMERS, Center for Superconductivity Research, Univ of Maryland, D.J. ARENAS, Dept of Physics, Univ of Florida, Y.J. WANG, NHFML, Florida State University, AMLAN BISWAS, D.B. TANNER, Dept of Physics, Univ of Florida — We report far-infrared temperature (300 K-20 K) and magnetic field (0-18 T) dependent reflectance and transmittance studies of 1000 A-thick hole-doped LPCMO thin films. Temperature-dependent measurements show evidence of phase coexistence in the sense that the film still shows insulating behavior at very low temperatures. Magnetic field studies at 4.2 K observe an insulator to metal transition, seen as large changes in reflectance and transmittance. The spectra are analyzed by using standard multilayer film-fitting procedures to extract the optical conductivity and other optical constants. The results are discussed in the context of effective medium approximations.

1Supported jointly by NSF grant DMR-0305043 and DOE contract DE-A102-03ER46070.

Thursday, March 8, 2007 8:00AM - 11:00AM

Session U14 GMAG DMP FIAP: Focus Session: Magnetization Dynamics and Half Metals

Colorado Convention Center Korbel 4D

8:00AM U14.00001 Theoretical limit of the minimal magnetization switching field and the shape of a field pulse for minimal reversal time of Stoner particles, X.R. WANG, Z.Z. SUN, The Hong Kong University of Science and Technology — The theoretical limit of the minimal magnetization switching field and the optimal field pulse design for uniaxial Stoner particles is investigated. Two results are obtained. One is the existence of a theoretical limit of the smallest magnetic field out of all possible designs. It is shown that the limit is proportional to the damping constant in the weak damping regime and approaches the Stoner-Wohlfarth (SW) limit at large damping. For a realistic damping constant, this limit is more than ten times smaller than that of so-called precessional magnetization reversal under a non-collinear static field, showing a big room for possible improvement in current available strategies. The other is on the optimal field pulse design. If the magnitude of a magnetic field does not change, but its direction can vary during a reversal process, there is an optimal design that gives the shortest switching time. The switching time depends on the field magnitude, damping constant and magnetic anisotropy. The two results can be used to evaluate various magnetization reversal strategies. Reference: Z.Z. Sun, and X.R. Wang, Phys. Rev. B 73, 092416 (2006); 74, 132401 (2006); Phys. Rev. Lett. 97, 077205 (2006).
8:12AM U14.00002 Coupled Precession Modes in Indirect Exchanged-Coupled Thin Films, STEVEN MICHALSKI, JIAN ZHOU, BOB BUCKLEY, RALPH SKOMSKI, ROGER KIRBY, Department of Physics and Astronomy and Nebraska Center For Materials and Nanoscience, University of Nebraska, Lincoln NE, 68588-0111 — Static and dynamic magnetic properties of exchange-coupled magnetic layers have been investigated by magneto-optical measurements. Our samples are [Pt/Co] multilayers with perpendicular magnetic anisotropy (PMA) exchange-coupled to a Co (Ni) layer with in-plane magnetic anisotropy by a variable thickness intervening Pt layer. The magnetic properties of such systems are controllable by tuning the exchange strength and PMA. To measure the magnetization precession, we use a femtosecond laser in a pump-probe experiment with direct optical excitation and preliminary measurements using a magnetic field pulse excitation. Both the strength and the angle of an external applied magnetic field were varied and for many samples, two modes with two distinct precession frequencies were observed, with frequencies that depend on the strength and the angle of the applied field. Our results are interpreted by a LLG-based model which predicts two modes whose behaviors depend on the strength and sign of the exchange coupling. This model is in a good qualitative agreement with our data and allows us to estimate the magnitude of the exchange coupling between the two layers. This work is supported by NSF-MRSEC, NCMN, and the W. M. Keck Foundation.

8:24AM U14.00003 Frequency-dependent magnetization response of CoFe thin film, MINGQIANG BAO, ALEXANDER KHTITIN, JOOYOUNG LEE, KANG L. WANG, EE Dept.., UCLA, AJEY P. JACOB, TMG External Programs, Intel Corporation — Frequency-dependent magnetization dynamics in CoFe thin films is investigated. Magnetization has been generated and detected by a pair of micrometer-wide antennas. The experimental data have been mapped showing the frequency-dependence of both the amplitude and the phase under external magnetic field. The response on a continuous single frequency excitation shows complex behaviors including those of harmonic resonances and half-frequency resonances. Furthermore, the device time-domain response of any input voltage/current pulse under any external magnetic field (below 350 Oe) can be reconstructed from our measured frequency-domain maps through the Fourier transform, and is validated with our time-domain measurement data.

*The authors would like to thank Dr. S. Wang and Dr DW Lee for growing CoFe thin-films. The work was supported in part by Western Institute of Nanoelectronics (WIN) and the Microelectronics Advanced Research Corporation (MARCO) Focus Center on Functional Engineered Nano Architectonics (FENA).

8:36AM U14.00004 Vortex Dynamics Imaged by Time-Resolved Scanning Transmission X-Ray Microscopy, HERMANN STOLL, Max Planck Institute for Metals Research, Heisenbergstr.3, 70569 Stuttgart, Germany — Substantial progress in the understanding of magnetic vortex dynamics has been achieved by implementing 100 ps time-resolved magnetic imaging techniques into a Scanning Transmission X-Ray Microscope (ALS, Berkeley, BL 11.0.2) with a lateral resolution of 20-40 nm. Gyrotropic vortex motion excited by in-plane alternating magnetic fields was studied in micron-sized ferromagnetic vortex structures. The vortex core, extending over a range of about 20 nanometers in the center of a vortex structure, plays a key role in vortex dynamics. We have been able to perform time-resolved imaging of the out-of-plane magnetization distribution of the excited vortex core. In addition, we have discovered new switching schemes to change the direction of the vortex core polarization in micron-sized ferromagnetic vortex structures, either (i) by altering the amplitude of an alternating magnetic field at a frequency close to the eigenfrequency of the gyrotropic vortex motion or (ii) by applying a short burst (e.g., one single period) of ac magnetic fields [1]. Magnetic vortex cores have already been discussed as candidates for magnetic data storage, but for the switching of their polarization large magnetic fields in the order of half a Tesla were required so far. The vortex core reversal schemes presented here need significantly lower magnetic fields (down to a few mT).

The switching mechanism as reproduced by micromagnetic simulations [1] involves: (i) creation of a vortex–antivortex pair, both with opposite polarisation and (ii) annihilation of the antivortex with the original vortex. At the end a vortex with opposite polarization remains.


9:12AM U14.00005 Highly-coherent magnetic vortex oscillations driven by a dc spin-polarized current, V.S. PRIBIAK, G.D. FUCHS, P.M. BRAGANCA, O. OZATAY, J.C. SANKEY, D.C. RALPH, R.A. BUHRMAN, Cornell University, I.N. KRIVOTOV, U.C. Irvine — While it has been demonstrated that dc spin-polarized currents can drive microwave spin–wave oscillations in magnetic multilayers via the spin-transfer torque (STT) effect [1], little is known about persistent STT-driven oscillations in strongly non-uniform systems. We report the use of STT to drive steady-state gigahertz-frequency oscillations of a magnetic vortex. We use an elliptical Py-Cu-Py nanopillar spin-valve structure in which one of the Py layers is sufficiently thick that its magnetization assumes a vortex configuration. The oscillations, which can be obtained in essentially zero applied field, are highly coherent, with full-widths at half maximum of less than 300 kHz at room temperature being obtained under certain bias conditions. We will discuss the observed sensitivity of the oscillation line-width to magnetic defects. We will also present measurements of the temperature-dependence of the oscillations, which we are pursuing to obtain a more complete understanding of how magnetic imperfections and thermal fluctuations determine the performance of this new type of non-magnetic STT oscillator. We will also discuss the use of STT-driven ferromagnetic resonance to examine the various magnetic modes that can be present in these nanoscale vortex structures. [1] S. I. Kiselev et al., Nature (London) 425, 380 (2003).

9:24AM U14.00006 Driven dynamic mode-splitting of magnetic vortices1, KRISTEN BUCHANAN, MARCOS GRIMSDITCH, FRANK FRADIN, SAM BADER, VÁL NOVOSAD, Center for Nanoscale Materials and Materials Science Division, Argonne National Laboratory — It has been established theoretically and experimentally that a magnetic vortex in restricted geometry possesses a translational excitation that corresponds to circular motion of the vortex core at a characteristic frequency. Here we explore the effect of increased driving-field amplitude on this dynamic mode using a microwave reflection technique. We find a new effect - the vortex translational eigenmode splits into two peaks. The splitting in frequency is >25% for driving magnetic fields <22 Oe for micron-sized permalloy ellipses that are 40-nm thick. Splitting effects were detected for driving fields as low as 3 Oe in circular dots. The magnetic vortex motion excited by in-plane alternating magnetic fields was studied in micron-sized ferromagnetic vortex structures. The vortex core, extending over a range of about 20 nanometers in the center of a vortex structure, plays a key role in vortex dynamics. We have been able to perform time-resolved imaging of the out-of-plane magnetization distribution of the excited vortex core. In addition, we have discovered new switching schemes to change the direction of the vortex core polarization in micron-sized ferromagnetic vortex structures, either (i) by altering the amplitude of an alternating magnetic field at a frequency close to the eigenfrequency of the gyrotropic vortex motion or (ii) by applying a short burst (e.g., one single period) of ac magnetic fields [1]. Magnetic vortex cores have already been discussed as candidates for magnetic data storage, but for the switching of their polarization large magnetic fields in the order of half a Tesla were required so far. The vortex core reversal schemes presented here need significantly lower magnetic fields (down to a few mT).

The switching mechanism as reproduced by micromagnetic simulations [1] involves: (i) creation of a vortex–antivortex pair, both with opposite polarisation and (ii) annihilation of the antivortex with the original vortex. At the end a vortex with opposite polarization remains.

1 This work was supported by DOE contract number DE-AC02-06CH11357. We acknowledge stimulating discussions with K. Guslienko.

9:36AM U14.00007 Electronic and magnetic properties of the La$_0.7$Sr$_{0.3}$MnO$_3$/SrTiO$_3$ interface from first principles calculations, HAND ZENIA, Department of Physics, Georgetown University, USA, GILLIAN GEHRING, Department of Physics and Astronomy, University of Sheffield, UK, WALTER TEMMERMAN, Daresbury Laboratory, Daresbury, Warrington, UK — We present results of first principles calculations of the electronic and magnetic properties of the La$_0.7$Sr$_{0.3}$MnO$_3$/SrTiO$_3$ interface. We are interested in the changes with respect to the bulk as concerns ferromagnetism and half-metallicity. The bulk calculations give a nearly half-metallic ground state for the manganite. In transport the system is predicted to be totally half-metallic. This latter property is preserved at the interface only if the magnetic coupling between the interface region and the bulk is ferromagnetic. We have looked at the two possible interface terminations between La$_0.7$Sr$_{0.3}$MnO$_3$ and SrTiO$_3$ and found that one of the interfaces preserves the bulk properties of La$_0.7$Sr$_{0.3}$MnO$_3$ whereas the other type of termination suppresses them. Reducing the number of holes at the interface by introducing La$_2$MnO$_3$ restores ferromagnetism. Hence the possibility of engineering interfaces to improve the Tunneling Magneto-Resistance yield in the La$_0.7$Sr$_{0.3}$MnO$_3$/SrTiO$_3$/La$_0.7$Sr$_{0.3}$MnO$_3$ tunnel junctions.

25% for
10:00AM U14.00009 Spin Polarization and Spin Transport in Co-based Heusler alloys, MUHAMMAD M. FAIZ, RAGHAVA P. PANGULURI, Wayne State University-Physics Department, SABINE WURMEHL, CLAUDIA FELSER, Johannes Gutenberg-Universität, Germany, BORIS NADGORNY, Wayne State University-Physics Department — The Co-based Heusler alloys are of special interest for possible spintronic applications due to their high Curie temperatures and high magnetic moment per unit cell. Co$_3$S$_2$Fe is especially promising as a candidate half-metal as it has a Curie temperature of approximately 1100K and the integer magnetic moment of 6\mu_B per unit cell [Ref. S. Wurmehl et al 1]. The samples have been prepared by arc melting of stoichiometric quantities of pure metals in argon atmosphere followed by annealing in sealed quartz tubes at 1300K. Here, we report comparative spin polarization, $P$, in Co$_3$FeSi and Co$_2$MnFeSi using Point Contact Andreev Reflection Spectroscopy (PCAR). We have also studied spin transport in Heusler/Au bilayers. Variable thickness Au films were deposited on top of the Heusler samples and the PCAR technique was then used to probe $P$ on the Au side. We will give the estimates of the spin diffusion length in Au based on these measurements and compare the results with conventional ferromagnetic spin injectors. 1. S. Wurmehl et al., J. Appl. Phys. 99, 08J103 (2006).

10:12AM U14.00010 A magneto-optical study of Heusler alloy Co$_2$MnGe films grown on Ge(111) substrates, PRANABA MUDULI, WIL RICE, BRIAN COLLINS, LIANG HE, FRANK TSUI, University of North Carolina at Chapel Hill — We report an extensive study of magneto-optic properties and magnetic anisotropy of ternary alloys of Co, Mn and Ge over a wide range of composition near the Heusler alloy compound Co$_2$MnGe grown on a single Ge(111) substrate by combinatorial molecular-beam epitaxy. The scanning magneto-optic Kerr effect (MOKE) study reveals a range of room temperature ferromagnetic phases near the Heusler alloy composition. A ridge of higher MOKE intensity near the Co/Mn atomic ratio of two is found, which appears to correlate with the structural perfection of the epitaxial film. The MOKE hysteresis loops in this composition range exhibit asymmetries that are associated with the presence of a large second-order magneto-optic effect. The magnetic anisotropy in the same composition range can be described by a combination of a six-fold and a uniaxial term. A single domain model in conjunction with the second-order MOKE is used to explain the magnetic anisotropy in these alloys. The model reveals a systematic change of magnetic anisotropy and the second-order MOKE coefficients as a function of composition and structural and chemical ordering of the films.

10:24AM U14.00011 The electronic band structure of Co$_2$S$_2$, NING WU, Dept. of Physics and Astronomy and the Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, YAROSLAV LOSOVYJ, Center for Advanced Microstructures and Devices, Louisiana State University, DAVID WISBEY, KIRILL BELASHCHENKO, Dept. of Physics and Astronomy and the Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln — We have identified a strongly dispersing band of Co$_2$S$_2$(100), with both sulfur and cobalt weight, along the Γ-X direction of the bulk Brillouin zone, from photon energy dependent angle resolved photoemission studies. From the critical points of the experimental band structure, the inner potential is estimated at about 4 to 5 eV, consistent with LEED I(V) analysis. The small inner potential indicates that Co$_2$S$_2$ has a narrow band width, consistent with the theoretical expectations. The clearly favored structural model from the LEED I(V) analysis is sulfur with cobalt terminated surface.

10:36AM U14.00012 Spin polarization of the ferromagnetic semimetal EuB$_6$, XIAOHONG ZHANG, STEPHAN VON MOLNAR, PENG XIONG, Department of Physics and MARTECH, Florida State University, ZACH FISK, Department of Physics, University of California at Irvine — Much progress has been made recently in the understanding of the electronic properties of EuB$_6$. However, the details of the electronic structure remain contentious. Several band structure calculations have produced different degrees of conduction-valence band overlap for the two spin subbands. In particular, some calculations predict a half-metallic band structure, i.e., 100% spin polarization at the Fermi level. We have performed direct measurements of the spin polarization of EuB$_6$ crystals using Andreev reflection spectroscopy. Planar junctions of EuB$_6$/Pb were fabricated on crystals grown with an Al flux method. The conductance spectra were measured using phase-sensitive detection at several temperatures below $T_C$ of Pb. The spectra are well-described by the spin-polarized BTK model. More than seven junctions were measured and a spin polarization of 55 ± 10% is obtained. Our results indicate that in ferromagnetic EuB$_6$, the electrons and holes at the Fermi level are not fully spin-polarized. This work was supported by a FSU Research Foundation PEG grant and NSF grant under DMR-0503360. 1. J. Kunes and W.E. Pickett, PRB 69, 165111 (2004); M. Kreisel and W. Nolting, PRB 72, 245117 (2005).

10:48AM U14.00013 Sharp switching of the magnetization in Fe$_{1+4}$TaS$_2$, EMILIA MOROSAN, HENNY ZANDBERGEN, LU LI, MINHUEA LEE, JOSEPH CHECKELSKY, MICHAEL HENRICH, THEO SIEGRIST, N. PHUAN ONG, ROBERT CAVA, Princeton University — Anisotropic magneto-transport measurements are reported on Fe$_{1+4}$TaS$_2$ single crystals grown by vapor transport. Both the magnetization and resistivity are extremely anisotropic, with the magnetic moments aligned parallel to the c crystallographic direction. Fe$_{1+4}$TaS$_2$ orders ferromagnetically below $T_C = 160$ K and displays very sharp hysteresis loops in the ordered state for H//c. The corresponding magnetoresistance is negative, and it qualitatively reproduces the features observed in the M(H) data, by showing a sharp drop around the critical field $H_C$ for the moment reversal. For field applied within the ab plane, the magnetization remains small and linear in field up to 5 T, and the magnetoresistance is positive and quadratic in field, with no visible hysteresis. The squareness of the M(H) loops and the high critical field for the magnetization switch ($H_{c2} = 3.7$ T at $T = 2$ K) allow us to classify Fe$_{1+4}$TaS$_2$ as a strong ferromagnet.

---

Session U22 GSNP DMP: Focus Session: Friction Colorado Convention Center 108
8:00AM U22.00001 Fundamental aspects of energy dissipation in friction , MIGUEL SALMERON, Lawrence Berkeley National Laboratory and Materials Science and Engineering Department, University of California, Berkeley — Energy dissipation in friction is mediated by excitation of elementary processes including surface phonons and electronic excitations. These excitations couple through anharmonic interactions or by Frank-Condon nuclear motions to bulk substrate phonons, which ultimately appear as heat. This gives rise to numerous phenomena including friction anisotropy, velocity dependence, and dissipative surface charge motion. Friction anisotropy can appear when phonon modes with specific polarizations are forbidden in particular crystal directions. Electronic excitations have been discussed and investigated but never clearly and definitely identified as primary mechanisms in contact friction. I will discuss these topics using recent experimental results in my laboratory including the large friction anisotropy of Al-Ni-Co decagonal quasicrystals, the role of hydrogen bonding networks in determining the velocity dependence of friction and finally the control of friction by changing the carrier concentration near the surface of p and n semiconductors.

8:36AM U22.00002 A nanotribology study of self-mated vs. unmated interfaces and local packing density effects for octadecyltrichlorosilane monolayers and silicon , ERIN FLATER, Luther College, W. ROBERT ASHURST, Auburn University, ROBERT CARPICK, University of Pennsylvania — We use atomic force microscopy (AFM) to determine the frictional properties of nanoscale single asperity contacts involving octadecyltrichlorosilane (OTS) monolayers and silicon. Quantitative AFM measurements are performed using both uncoated and OTS-coated silicon AFM tips and surfaces. Friction is reduced by the presence of the OTS coating, and the overall shape of the friction vs. load plot strikingly depends on whether or not the substrate is coated with OTS, regardless of tip material. Uncoated substrates exhibit the common sublinear dependence, while coated substrates exhibit an unusual superlinear dependence. These results can be explained qualitatively by invoking molecular plowing as a significant contribution the frictional behavior of OTS. Direct in-situ comparison of two intrinsic OTS structural phases of otherwise identical molecules on the substrate show that the lower packing phase density exhibits higher friction, decisively observed here in single, uninterrupted images on the same monolayer for the first time. The lateral stiffness of the two OTS structural phases is indistinguishable, which implies that the packing density directly affects the interface’s intrinsic resistance to shear as opposed to simply modifying the stiffness of the monolayer.

8:48AM U22.00003 Dynamical noise and avalanches in quasi-static plastic flow of amorphous solids , ANAEL LEMAITRE, Institut Navier, CHRISTIANE CAROLI INSP, Universite Pierre et Marie Curie-Paris 6, Universite Denis Diderot-Paris 7 — We build a mean-field model of plasticity of amorphous solids, based on the dynamics of an ensemble shear transformation zones, interacting via intrinsic dynamical noise generated by the zone flips themselves. We compare the quasi-static, steady-state properties for two types of noise spectrum: (G) Gaussian; (E) broad distribution derived from quadrupolar elastic interactions. We find that the plastic flow proceeds via avalanches whose scaling properties with system size are highly sensitive to noise tails. Comparison with available data suggests that non-affine strain fields might be of paramount importance in the small systems accessible to molecular simulations.

9:00AM U22.00004 Dynamics of Phononic Dissipation at the Atomic Scale1, Haldun Sevincli, Somay MUKHOPADHAY, R. TUGRUL SENGER, SALIM CIRACI, Department of Physics, Bilkent University — Dynamics of dissipation of a local phonon distribution to the bulk is a key issue in boundary lubrication and friction between sliding surfaces. We consider a highly excited molecule which interacts weakly with the substrate surface. We study different types of coupling and substrates having different types of dimensionality and phonon densities of states. We propose three different methods to solve the dynamics of the combined system, namely the equation of motion technique, Fano-Anderson method and the Green’s function method. Using this theoretical framework we present an analysis of transient properties of energy dissipation via phonon discharge at the microscopic level. The methods allow the theoretical calculations to be extended to include any density of states for the substrate including experimental ones and any type of molecule that represent the lubricant or the aspereity.

9:12AM U22.00005 Friction and Viscous Forces in Sub-Nanometer Water Films1, TAI-DE LI, ELISA RIEGO, School of Physics, Georgia Tech, SCHOOL OF PHYSICS, GEORGIA INSTITUTE OF TECHNOLOGY TEAM — Water under nano-confinement is ubiquitous, with examples including clay swelling, aquaporines, ion channels, and water menisci in micro-electrical-mechanical-systems. However, the structural and rheological characteristics of nano-confined pure and ionized water continue to be the subject of discussion and debate. Here, we report an experiment in which an atomic force microscope tip approaches a flat solid surface in purified water, while small lateral oscillations are applied to the tip. Direct measurements of the lateral forces encountered by a nano-size tip approaching a solid surface in purified water are reported for tip-surface distances, 0 < 0.03 nm < d < 2 nm. We find that, for hydrophilic surfaces, the dynamic viscosity is measured to grow up orders of magnitude in respect to bulk water, whereas no significant increase in the viscosity has been detected when the confining solid surface is hydrophobic. The origin of the observed different behavior is discussed.

9:24AM U22.00006 Friction Reduction Using Self-Assembled Hydrogels , MICHAEL J. MACKEL, JULIA A. KORNFIELD, California Institute of Technology — Friction of agarose-based hydrogels against bare glass is examined as a function of added linear polyelectrolyte using a stress rheometer to measure the angular velocity of a clean glass plate against the hydrogel surface as a function of applied torque and normal force. Incorporating linear dextran sulfate into 2 weight percent agarose hydrogel reduces friction on the hydrogel surface. The reduction of friction is a nonmonotonic increase in the viscosity has been detected when the confining solid surface is hydrophobic. The origin of the observed different behavior is discussed.

9:36AM U22.00007 High velocity sliding at a compressed Al(111)/Al(100) interface1, J. E. HAM-MERBERG, Los Alamos National Laboratory, R. RAVELO, University of Texas, El Paso, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — We discuss high velocity sliding at a compressed Al(111)/Al(100) interface sliding in the 1T0 direction at a pressure of 15 GPa. Three temperatures are considered, T=232, 464 and 696 K. System sizes are 1.41014 atoms. We find that for velocities above a critical velocity, v_c, the frictional force scales as (v/v_c)^-beta with \beta \approx 3/4. We discuss the temperature and size dependence of v_c. We find that below v_c the frictional force is an increasing function of velocity with an initial linear dependence. Above v_c there is a regime of interfacial instability characterized by a (100) transformation front moving into the (111) material. This is followed by a fluid regime for which a Coutte flow profile develops at the interface, the thickness of which grows with increasing velocity.

1This work supported by the Department of Energy under contract W-7405-ENG-36

9:48AM U22.00008 The Dynamics of Precursors to Frictional Sliding , JAY FINEBERG, SHMUEL RUBIN-STERN, GIL COHEN, The Hebrew University of Jerusalem — The dynamics of frictional motion are governed by the nature of the interface separating two sliding materials. We report that the spatial profile of the contact area along an interface this quantum which evolves via a discrete sequence of rapid crack-like precursors to overall motion. These precursors, which are generated at stress levels much lower than the critical stress for sliding, significantly modify the initially uniform contact area profile. Thus, when overall sliding finally occurs, the contact area is highly non-uniform in space. These results suggest a fundamentally new view of the processes leading to frictional motion with ramifications to earthquake dynamics and material failure.
10:12AM U22.00010 Molecular Dynamics Simulation of Frictional Melting, SHIGENOBU HIROSE, The Earth Simulator Center, JAMSTEC — Frictional melting produces lubricant at the sliding plane and changes the physics of dynamical sliding, which may play a key role on coseismic slipping. In this paper, molecular dynamics simulation is used to study the basic physics of frictional melting. Here, friction between a Lenard-Johns material and a rigid material is considered for simplicity. When the sliding velocity is low enough, there is no melting and the friction coefficient almost does not depend on the sliding velocity. On the other hand, when the sliding velocity is so high that frictional melting occurs, the friction coefficient decreases due to the melting lubricant. A preliminary result shows that the friction coefficient is roughly power-law of the sliding velocity. A discussion will also be given on the thermodynamic balance between the frictional heating, cooling by latent heat, and conduction cooling.

10:24AM U22.00011 Molecular Dynamics Simulations of Nanotribology with Accurate Probe Tip Models, MICHAEL CHANDROSS, Sandia National Laboratories, CHRISTIAN LORENZ, Iowa State University, GARY GREST, Sandia National Laboratories — Results for extensive dynamical nanotribological simulations of amorphous silica tips in contact with alkylsilane self-assembled monolayers (SAMs) will be presented. The radius of curvature of the tips match experimental dimensions. Comparison with contact mechanics models indicate that the standard JKR and DMT models do not give the correct dependence of contact area on applied force. The dependence of the tribological response on the chain length of the SAM has been determined. For short chains and for long chains at low loads the SAM presents a disordered sliding surface to the tip and the chain length is irrelevant. This result is in agreement with our previous simulations for SAMs in contact with a flat surface. For longer chains at higher loads the tip penetrates the monolayer and the friction is dominated by a plowing mechanism. Sandia is a multiprogram laboratory operated by Sandia Corp., a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Thursday, March 8, 2007 8:00AM - 11:00AM — Session U25 DPOLY DMP: Organic Field-Effect Transistors Colorado Convention Center 203

8:00AM U25.00001 Intrinsic transport anisotropy in single-crystal FETs on new rubrene derivatives, A.F. STASSEN, W. KALB, S. HAAS, ETH Zurich, U. BERENS, H.J. KIRNER, Ciba SC Inc., Switzerland, B. BATLOGG, ETH Zurich — For the charge transport in a field-effect transistor (FETs), both the spectral density of gap states and the intrinsic mobility play a critical role. The latter is closely related to the arrangement of the molecules in the solid. We present measurements on FETs fabricated on single crystals of new rubrene derivatives. One of them crystallizes in two polymorphic forms: One polymorph shows a very high field-effect mobility (>10 cm²/Vs) and a transport anisotropy which can be directly related to the crystal packing. In the second polymorph, the same molecules are arranged in a different structure with minimal π-overlap. No charge transport could be induced, highlighting the crucial role played by the wave-function overlap associated with the packing.

8:12AM U25.00002 RC Transmission Line Characterization of Organic Thin Film Transistors, DANIEL LENSKI, ADRIAN SOUTHARD, MICHAEL S. FUHRER, Department of Physics and Center for Superconductivity Research, University of Maryland, College Park, MD 20742, USA — The transport properties of organic semiconductors are typically measured in a field-effect transistor geometry with DC gate and drain bias. We have developed a novel method of characterizing organic thin films using a 2- or 3-contact transmission line configuration, in which an AC voltage is applied to the thin film and the phase and magnitude of the current are measured. This method can determine both sheet resistance and contact resistance. Additionally, this method may reveal inherent frequency-dependent transport properties of organic semiconductors, which may be significant for future applications of these materials. We present the results of transmission line measurements of pentacene thin films, and compare them to transport data obtained from FET characterization. This work has been supported by the Laboratory for Physical Sciences.

8:24AM U25.00003 Eliminating gate bias stress effects in organic field-effect transistors, WOLFGANG L. KALB, THOMAS MATHIS, SIMON HAAS, ARNO F. STASSEN, BERTRAM BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — We report on organic field-effect transistors with unprecedented resistance against gate bias stress. The single crystal and thin-film transistors combine small molecule organic semiconductors and an organic gate dielectric with a remarkable electrical breakdown strength. The single crystal devices have no current hysteresis. Extended gate bias stress leads to almost unmeasurable changes in the transfer characteristics: the induced interface state density is of order 10^7/cm². In contrast, stress-induced trap densities of order 10^13/cm² have been identified previously in devices with SiO₂ or OTS-treated SiO₂ gate dielectrics. Therefore, adverse gate bias stress effects are not generic to oligocene organic semiconductors, and there is no conceptual limitation for the stability of organic-based transistors in contrast to hydrogenated amorphous silicon.

8:36AM U25.00004 Field dependent hole transport mobility studies on a select group of conjugated polymers, N.C. HESTON, B. WILSON, E. M. GALAND, D. B. TANNER, J. R. REYNOLDS, University of Florida — The thin film hole transport properties of a set of cyanovinylene-linked 3,4-propylenedioxythiophene (ProDOT)/dialkoxyphenylene polymers, and regioregular poly(3-hexylthiophene), were measured by fabricating hole dominated devices and measuring the room-temperature I-V characteristics. The data were fitted to a model of field-dependent space-charge-limited current. By carrying out both the fabrication and the measurements inside an inert atmosphere we attained significant improvements to the reproducibility of our results. We also found that exposing the devices to heating increased the field dependent hole mobilities of the polymers with values ranging from 5.2 x 10^-7 (cm²/Vs) to 3.1 x 10^-6 (cm²/Vs).
9:48AM U25.00005 Electric Field Induced Conductivity of Disorder Driven Anderson Insulator$^1$. VLADIMIR PRIGODIN, ARTHUR EPSTEIN, Ohio State University — The effect of an electric field on the Anderson localization is considered. In the 3d case the field mixing the localized and extended states leads to delocalization. In the 2d case, the localization exponentially weakens with increasing kinetic energy so that in principle any field leads also to total delocalization. The field induced IMT occurs in the 1d case [1]. However, the delocalization effect of field on the Anderson insulator hardly is observable because it is masked by phonon assisted hopping. In the localized phase for each localized state along the field there remain remote empty states whose energies are lower and electrons hop to those states by emission of phonons. Therefore the electric field induces the crossover in temperature dependence of hopping conductivity from activation (variable range hopping conductivity) to emission (metallic like conductivity) regime. The results have implications for the recent studies of field effects in polymer based transistors [2].


9:00AM U25.00006 Device Model for Organic Semiconductor Light-Emitting Field-Effect Transistors, DARRYL SMITH, Los Alamos National Laboratory, P. PAUL RUDEN, University of Minnesota — Recent experiments demonstrate ambipolar channel conduction and light generation in polymer field effect transistors (FETs).$^{1,2}$ In the ambipolar mode of operation, the gate potential lies between those of the source and drain contacts, hence electrons are injected from one of these contacts and holes from the other. The carriers recombine in channel regions where both types of carriers are present, and the location of the resulting light emission is controlled by the voltages applied to the terminals. We describe the device model for ambipolar organic FETs based on the gradual channel approximation. Trapping of injected carriers in localized states within the polymer energy gap is shown to be important. A non-linear differential equation for the channel potential is derived and solved numerically. Carrier density and recombination profiles are determined. The calculations are in good agreement with experimental data.$^{1,2}$


9:12AM U25.00007 Electrostatic Injection of Very Large 2D Charge Carrier Densities to Obtain Metallic Conductivities in Organic Semiconductors, MATTHEW PANZER, C. DANIEL FRIEBIE, University of Minnesota — The traditional choice of SiO$_2$ for the gate dielectric material in organic field-effect transistors (OFETs) limits the amount of charge that one can induce via the field effect due to its relatively weak dielectric strength. In fact, the maximum 2D charge density achievable (near SiO$_2$ breakdown, typically $>$ 100 V applied) is only $\sim$10$^{12}$ charges/cm$^2$, while the 2D molecular packing density of many common organic semiconductors is on the order of 5 x 10$^{14}$ molecules/cm$^2$. In order to achieve a higher fraction of charged semiconductor molecules in the 2D OFET channel, a dielectric layer with a higher capacitance is required. We have used a solid polymer electrolyte as an OFET dielectric in order to obtain 2D charge densities exceeding 10$^{14}$ charges/cm$^2$ at operating voltages under 3 V in a variety of organic semiconductors. We have observed metallic conductivity values ($\sim$1000 S/cm) and nearly temperature-independent resistance ratios in poly(3-hexylthiophene) films using a polymer electrolyte-gated OFET. In addition, conductivity maxima at carrier densities approaching 1 charge/molecule were observed in oligomeric, polymeric, and single-crystal organic semiconductor materials. This phenomenon may be caused by carrier correlations or a complete emptying of the semiconductor transport band at very high charge densities.

9:24AM U25.00008 Charge mobility of discotic mesophases of hexabenzocoronene derivatives: a multiscale quantum/classical study of the effects of side chain substitution$^3$. DENIS ANDRIENKO, VALENTINA MARCON, KURT KREMER, Max-Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, JAMES KIRKPATRICK, JENNY NELSON, Department of Physics, Imperial College London, Prince Consort Road, London SW7 2BW, United Kingdom — Discotic liquid crystals form columnar phases, where the molecules stack on top of each other and the columns arrange in a regular lattice. The self-organization into stacks results in the one-dimensional charge transport along the columns. Using atomistic molecular dynamics (MD) simulations we study the solid and liquid crystalline columnar discotic phases formed by the alkyl-substituted hexabenzocoronene mesogens. Correlations between the molecular structure, packing, and dynamical properties of these materials are established. Combining Kinetic Monte Carlo and MD trajectories a correlation between the material morphology and charge mobility is then obtained. We are able to reproduce the trends and magnitudes of mobilities as measured by pulse-radiolysis time-resolved microwave conductivity technique.

3 supported by DFG via IRTG between Germany and Korea. VM acknowledges AvH Foundation. JK acknowledges EPSRC.

9:36AM U25.00009 The electronic structure and charge carrier dynamics in organic molecular crystals$^1$, NA SAI, The University of Texas at Austin, ZHIQIANG LI, University of California, San Diego, VITALY PODZOROV, Rutgers University, MICHAEL MARTIN, Lawrence Berkeley National Laboratory, MICHAEL GERSHENSON, Rutgers University, DIMITRI BASOV, MASSIMILIANO DI VENTRA, University of California, San Diego — Organic molecular crystal semiconductors have been receiving intense attention recently. The much higher carrier mobility and intrinsic physical properties uncovered in these materials offer many fundamental advantages over their polycrystalline counterpart. Combined with infrared absorption studies of the rubrene based field effect transistor, we study the intrinsic anisotropy in the basal a-b plane of the rubrene crystal. We report the structure and electron structure of the rubrene crystals using density-functional theory. We find fairly light effective masses of the order of the free electron mass, in agreement with those extracted from infrared measurements. In light of these results, we discuss possible mechanisms of charge transport in these crystals.

1 Work supported by NSF.

9:48AM U25.00010 Analysis of the Injection Efficiency Saturation in Polyfluorene Copolymers, DAVID DUNLAP, University of New Mexico, TIANJIAN LU, HON HANG FONG, GEORGE MALLIARAS, Cornell University — Recent experiments of the transport of holes across a 1 - 5 μm layers of the copolymer poly[9,9-diocystylfluorenyl-2,7-diyl]-co-(4,4'-N-(4-sec-butyphenyl)di phenylamine)] (TFB) reveal an injection efficiency that saturates at high voltages, which is indicative of space-charge-limited current. The injection efficiency is on the order of 10$^{-3}$, three orders of magnitude smaller than what would be expected if the current followed the Mott-Gurney law. It is difficult to explain this behavior as arising from trapping phenomena, for time of flight transients show clear plateaus, and the extracted mobility is only weakly dependent on temperature$^1$. We propose that the behavior may be accounted for by an interface dipole at the metal/organic injecting contact which is dependent on the applied voltage. Quantitative support to for this mechanism is obtained through numerical simulations of the convection-diffusion equation.

10:00AM U25.00011 High-resolution electrical characterization of polyaniline/p-type organic semiconductor interfaces in thin-film transistors

KWANG SEOK LEE, TIMOTHY J. SMITH, University of Texas at Austin, CHRIS ZANGMEISTER, National Institute of Standards and Technology, JOUNG EUN YOO, KEITH J. STEVENSON, YUEH-LIN (LYNN) LOO — While the work functions of polyaniline (PANI) and gold are known to be similar (ca. 5 eV), we found the electrical properties of PANI/ and gold/p-type organic semiconductor interfaces in diethylenetriophene (DHT-Ant) and pentacene thin-film transistors (TFTs) to be significantly different. Specifically, the current-voltage (IV) characteristics of DHT-Ant TFTs with PANI show electron crowding in the saturation regime. Such current crowding is absent in DHT-Ant TFTs with gold electrodes. Surface potential measurements reveal reduced potential drops at the gold/DHT-Ant interface, relative to the PANI/DHT-Ant interface suggesting limited hole injection into DHT-Ant from PANI. In contrast, pentacene TFTs with PANI electrodes show near-ideal IV characteristics and negligible surface potential drops at the electrode/channel interface, whereas pentacene TFTs with gold electrodes exhibit significant potential drops at the electrode/channel. Hole injection thus appears to be more efficient from PANI than gold in pentacene TFTs, which can be directly correlated with the similar pentacene grain size and the identical fused ring orientation across the PANI/channel interface.

10:12AM U25.00012 Polymer LED interfaces studied with resonant soft x-ray reflectivity.

CHENG WANG, B. WATTS, T. ARAKI, H. ÄDE, NCSU, A. HEXEMER, A. GARCIA, T.-Q. NGUYEN, K.E. SOHN, J.E. KRAMER, UCSB — Multilayered polymer structures produced by alternate spin casting from polar and non-polar solvents are promising for polymer light emitting diodes (PLEDs). The structure of the interface between the active layers most likely significantly affects the device efficiency, yet little is known about the interfacial structure and how it affects properties of such devices. Recently, it has been shown that Resonant Soft X-ray Reflectivity (RSoXR) is an excellent tool to study polymer thin films without the need for deuteration. RSoXR can enhance the sensitivity to a particular interface by using specific photon energies. We have used RSoXR and characterized the interfacial width of bilayers of poly[2-methoxy-5-(2-ethylhexyl oxy)-p-phenylene vinylene] (PFNBr), materials relevant to PLED devices. MEH-PPV is a neutral conjugated polymer spin-cast from tolune (non-polar solvent) and PFNBr is a charged conjugated polymer (conjugated polyelectrolyte) spun-cast from methanol (polar solvent). Bilayers nominally 20 nm/80 nm PFNBr/MEH-PPV and 80 nm/20 nm MEH-PPV/PFNB were investigated and their interfacial widths were determined to be 1.3 and 1.4 nm, respectively.


YU CHEN, MASAYA NISHIOKA, ALLEN GOLDMAN, School of Physics and Astronomy, University of Minnesota, YU XIA, DANIEL FRISBIE, Department of Chemical Engineering and Material Science, University of Minnesota — Modulated organic field-effect transistors (FET) of rubrene were made by laminating organic single crystals on the top of two-dimension quantum dots arrays. By introducing the single crystal under-layer dots arrays, we were able to effectively separate organic crystals into mesoscopic-sized grains and reduced the density of trapping sites. Comparing with the conventional organic FETs, these structures show an enhanced mobility at low temperature. This was exhibited as a sharp increase in mobilities when temperature decreased below a characteristic temperature.

10:36AM U25.00014 Viewing density of states of the contact in organic thin-film transistors

TAKEO MINARI, KAZUHITO TSUKAGOSHI, TETSUHIKO MIYADERA, RIKEN/CREST, HIROMI ITO, RIKEN, YOSHINOBU AOYAGI, RIKEN/CREST, RIKEN/CREST TEAM — The large contact resistance is one of the most critical issues in the research and development of organic thin-film transistors (OTFTs). In this study, we developed a method for evaluating the injection process of OTFTs through the effective use of gate voltage dependence as energetic spectroscopy of charge injection. This spectroscopy, quasi-Fermi level tuning in contact by scanning the gate voltage provides essential clues to the determination of the energy state of the contact. Based on the concept that the contact resistance is composed of the resistance of a barrier at metal/organic interface and bulk resistance of organic film itself, we attempted to reduce the interface barrier height by inserting a thin doping layer of charge-transfer molecule (CTM) into the metal/organic interface. A suppression of the interfacial barrier height unveiled energetic distribution of the density of states (DOS) localized at the contact. We also found that the bulk transport clearly obeys the Meyer-Neldel rule, according to which the exponential density of states near the band edge limits the charge injection.

10:48AM U25.00015 ABSTRACT WITHDRAWN —

Thursday, March 8, 2007 8:00AM - 10:48AM —
Session U27 DMP DCOMP: Focus Session: Computational Nanoscience VII-Reactions on Surfaces and Nanostructures Colorado Convention Center 301

8:00AM U27.00001 Effects of Rh coordination and surface strain on NO dissociation

STEFANO DE GIRONCOLI, PUSHPA RAGHANI, SISSA, Trieste, Italy, PRASENJIT GHOSH, SHOBHANA NARASIMHAN, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — The Rh(100) surface is known to be a good catalyst for the reduction of NO. We try to understand the effect of Rh coordination and in plane strain on NO adsorption and its dissociation. To distinguish between the strain effects and charge transfer we look at the adsorption and dissociation of NO on Rh(100) and stretched Rh(100), in addition to NO adsorption on 1 ML of Rh/MgO at MgO and Rh lattice constants. As expected, we find that the adsorption energy of NO increases with reduction in effective coordination of Rh, i.e., while going from Rh(100), to stretched Rh(100), to 1 ML Rh/MgO, to 0.25 ML of Rh/MgO. In the case of NO on Rh(100) and on 1 ML Rh/MgO at lattice constant, we find that NO absorbs vertically at the bridge site between two Rh atoms; whereas, in the case of stretched Rh(100) and 1 ML of Rh/MgO at MgO lattice constant, NO absorbs horizontally at the hollow site. Hence, as the effective Rh coordination is changed, both adsorption geometries and adsorption energies change in a systematic way. This has an influence on the energetic barriers for the rate-limiting step in the reduction of NO on these surfaces.

8:12AM U27.00002 Bridging the materials gap in catalytic kinetics via first principles coarse-grained kinetic Monte Carlo simulations

ALTAF KARIM, DION VLACHOS, University of Delaware — We describe a first principles coarse-grained kinetic Monte Carlo technique enabling us to simulate catalysis under different technologically relevant conditions. By implementing coarse-grained KMC, various simulations are performed efficiently at much larger time and length scales. Using this approach, we studied catalytic oxidation of CO on different metal surfaces. Especially, we tried to understand the role of defects in catalytic kinetics such as steps, kinks, and multiple facets. These studies led us to some interesting results bridging the material gap in catalysis.
8:24AM U27.00003 Formation of Pt nano-islands on Ru(0001) surface: insights from ab initio calculations. 1, TALAT S. RAHMAN, University of Central Florida, MARISOL ALCANTARA ORTIGOZA, Kansas State University, SERGEY STOLBOV, University of Central Florida. — As reported [1], Ru nanoparticles with sub-monolayer of Pt are much more efficient catalysts for hydrogen oxidation than anodes used in standard fuel cells. Since this effect apparently depends on the size of Pt islands, we have performed density functional theory based calculations of energetics of Pt islands of varying size on the Ru(0001) surface. We find the formation energy of the island per atom to decrease monotonically from -5.1 eV to -6.1 eV, as the number of Pt atoms in the 2D island increases from one atom to one monolayer. Propensity of the systems to increase the number of interatomic bonds thus overpowers the effect of the stress caused by the 2.6% misfit of Ru and Pd interatomic bonds. As a result, Pt atoms prefer to coalesce on Ru(0001) increasing the cluster size up to one monolayer, in agreement with experimental data. This raises the question whether the key role of nano-sized Ru clusters [1] is to prevent coalescence of Pt islands by restricting their diffusion through facet edges. To address this issue we consider the effect of surface steps on Ru(0001) on the Pt island formation. 1. S. R. Brankovic, et al., Electrochem. Sol.-St. Lett. 4 (12) A217-A220 (2001).

1Work supported by DOE under grant No. DE-FG02-07ER46354.

8:36AM U27.00004 First principles studies of CO adsorption and diffusion over Pt nano-islands on Ru(0001) surface. 1, SERGEY STOLBOV, University of Central Florida, MARISOL ANCANTARA ORTIGOZA, Kansas State University, TALAT S. RAHMAN, University of Central Florida — Proton exchange fuel cells are promising tools for hydrogen economy. However, CO, present in hydrogen, blocks active Pt sites of anode that poisons its reactivity. As reported [1], small coverage of Pt on Ru nanoparticles is much less sensitive to CO than commercial catalysts. To understand this effect, we have performed density functional theory based calculations of the energetics of adsorption and diffusion of CO on the 7Pt-atom islands and on the Ru(0001) substrate. We find that CO adsorption energy increases as it moves from the center of the Pt island to its edge and further onto substrate. CO thus tends to move from the Pt island to the Ru substrate. Diffusion barriers are found to be lower than 0.3 eV suggesting this process to be fast. This finding suggests that this hydrogen oxidation catalyst is CO tolerant because of the propensity of CO to move from active Pt island site to the Ru substrate. We present the rationale for this effect using insights from detailed electronic structure calculations. [1] S. R. Brankovic, et al., Electrochem. Sol.-St. Lett. 4 (12) A217-A220 (2001).

1Work supported by DOE under grant # DE-FG02-07ER15842 and TeraGrid grant # TG-DMR050035N.

8:48AM U27.00006 Mechanism of the Energy Barrier Formation during Dissociation of Hydrogen Molecule on Mg(0001). SHIGEYUKI TAKAGI, KAZUO TSUMURAYA, Meiji University, JAPAN. — There has been no clear explanation on the mechanism of the energy barrier for the dissociation of the hydrogen molecules on the metal surfaces. When the hydrogen molecule approaches the surface of metals, the molecule dissociates and forms a new bond with the atoms on the surfaces. During the process the energy barrier appears on the Au or Cu or Mg surface, although no barrier appears on the Pt or Ni surface. Although the stability of hydrogen atoms has been clarified by use of the density of state,[1] there has been no clear explanation on the mechanism of the barrier formation. In the present paper we use a density functional calculation method to evaluate the charges that belong to the hydrogen atoms during the dissociation process of the hydrogen molecule on the Mg(0001) using Bader analysis. During the barrier formation, the charge transfers from the Mg substrate to the dissociating hydrogen atoms. We will discuss how this energy barrier can be explained with the sum of the independent systems of the electron donated Mg surface and the electron received hydrogen molecule. [1] B.Hammer and J.K.Nørskov, Nature 376, 238(1995).

9:00AM U27.00007 Theoretical study of tunneling spectra of tetramantane on Au(111) surface. EMMANOUIL KIOUPAKIS, Y. WANG, R. YAMACHIKA, X. LU, M. F. CROMMIE, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Diamondoids are a class of carbon-based molecules in which the carbon atoms are structured in a diamond-like fashion with all dangling bonds saturated with hydrogen atoms. Recently, scanning tunneling microscopy experiments were carried out to study the tunneling spectra of tetramantane on Au(111) surface. The elastic tunneling images have a LUMO-like character in a broad energy range around the Fermi level, while the inelastic signal shows spatial localization. We use ab-initio density functional theory calculations to study the molecule-surface system and discuss the observed elastic and inelastic tunneling spectra. This work was supported by National Science Foundation Grant No. DMR04-39768, by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and by an NSF Graduate Research Fellowship. Computational resources have been provided by NERSC and NPAI.

1Fellow of the “Alexander S. Onassis” Foundation

9:12AM U27.00007 Motion of clusters on complex surfaces. 1, SABRI ALKIS, JEFFREY KRAUSE, HAI-PING CHENG, University of Florida, Gainesville, FL, 32611-8435 — Polymer and organic molecule assemblies have been investigated intensely in the past decade, due to their vast range of applications in nano-molecular electronics and as bio-sensors. In particular, self-assembled monolayers (SAMs) of alkanethiol on the Au(111) surface are used widely in surface studies because they are simple structurally, stable thermodynamically and have well-defined order. In this project, inspired by recent experiments, we use classical molecular dynamics simulations to study motions of Agx clusters with various sizes on the alkanthiol SAMs. We report detailed results on dynamics, diffusion, and sintering processes of these nano-clusters.

1Acknowledgement: This work is supported by DOE under grant number DE-FG02-02ER45995

9:24AM U27.00008 Effects of water on the reactivity and stability of SiO2 nanostructure. 1, YAO HE, CHAO CAO, HAI-PING CHENG, University of Florida. — To investigate effects of water on the reactivity and stability of SiO2 nanostructure, we have performed first-principles molecular dynamics simulations of SiO2 nano-chain and nano-rod. The SiO2 nanostructures, which have stimulated many current research endeavors, can react with water strongly under internal or external stress. In our study, water monolayer films that cover the entire system are used to study the collective motion of protons. Structure, charge separation, stress dependent bond breaking and formation, and proton conduction are discussed based on results obtained at room temperature. Finally, we extend our effort to carbon nanotubes.

1NSF/DMR/ITR under grant DMR-0325553

9:36AM U27.00009 Enantiospecific adsorption of chiral molecules on chiral Au clusters. IGNACIO L. GARZON, XOCHITL LOPEZ-LOZANO, LUIS A. PEREZ, Universidad Nacional Autonoma de Mexico. — Enantioselectivity in gold clusters is investigated by studying the adsorption of a chiral amino acid (cysteine) on a chiral Au55 cluster using density functional calculations. The highest adsorption energies were found when the amino and thiolate functional groups of cysteine are bonded to the lowest coordinated edges of the chiral cluster. Enantiospecific adsorption is primarily obtained from the different bond location and strength, at the cluster edge, of the carbonyl groups forming the left- and right-handed enantiomers. These results provide theoretical support to convey enantioselectivity in asymmetric nanocatalysts using chiral gold clusters.
Spin-dependent electronic structure of transition-metal atomic chains adsorbed on single-wall carbon nanotubes

We present a systematic study of the electronic and magnetic properties of transition-metal (TM) atomic chains adsorbed on the zigzag single-wall carbon nanotubes (SWNTs). We examine the effect of the TM coverage and geometry on the binding energy and the spin polarization at the Fermi level. All those adsorbed chains studied have ferromagnetic ground state, but only their specific types and geometries demonstrated high spin polarization near the Fermi level. Their magnetic moment and binding energy in the ground state display interesting variation with the number of d electrons of the TM atom. Spin-dependent electronic structure becomes discretized when TM atoms are adsorbed on finite segments of SWNTs. Once coupled with nonmagnetic metal electrodes, these magnetic needles or nanomagnets can perform as spin-dependent resonant tunneling devices. Our study is performed by using first-principles pseudopotential plane wave method within spin-polarized density functional method. Reference: E. Durgun and S. Ciraci. Phys Rev B 74, 125404 (2006).

Ab initio study of adenine and thymine adsorption on carbon nanotubes

We have calculated hydrogen dissociation on Pd-doped single-walled carbon nanotubes using density functional theory. Our results show that the hydrogen dissociation is barrier-less on edge of Pd cluster, while on the top of Pd cluster the molecule would not automatically dissociate. Calculations also show that a dense doping with Pd cluster would modify the band structure of CNT substantially such that the doped tube becomes a semi-metal. The dissociation of hydrogen molecule will further change it into a semiconductor. Our NEGF calculations confirmed the band structure calculation, and suggested that Pd-doped CNT could be used as a hydrogen sensor device by measuring the conductance change of the device induced by hydrogen dissociation.

Dynamics and shape fluctuations of nanosized water pools in reverse micelles

Reverse micelles are surfactant assemblies containing nanosized water reservoirs which can serve as confined media for studying chemical reactions as well as for nanoparticle synthesis. Molecular dynamics simulations are performed for reverse micelles formed by the surfactant CTAB (Cetyl Trimethyl Ammonium Bromide) in cyclohexane with the cosurfactant pentanol. We present results for the dynamics of confined water and for shape fluctuations of the reverse micelles which can be probed experimentally using terahertz time-domain spectroscopy.

First-Principles Studies of sila-Diamondoids

We have developed new materials based on chemically modified graphene (CMG) sheets. By working with aqueous colloidal suspensions of "graphene oxide" sheets (graphene sheets that are oxidized) we have prepared individual CMG sheets deposited on substrates designed for optical characterization of them. We have also measured the physical properties of individual CMG sheets (i) fabrication & properties of ceramic composites with embedded CMG sheets (iv) fabrication of novel "paper-like" materials (analog: bucky paper) comprised of aligned CMG sheets and having thicknesses from less than 1 up to 20 micrometers. Here, we provide a broad overview of this work and also very briefly discuss our preliminary studies from NASA (\# NCC-1-02037) through the URETI on Bio-inspired Materials, the Naval Research Laboratory (\#N00173-04-2-C003) and the NSF (CMS-0510212), is appreciated.

The Structure of Suspended Graphene

The recent discovery of graphene has sparked significant interest, which has so far been focused on the peculiar electronic structure of this material, in which charge carriers mimic massless relativistic particles. However, the structure of graphene is also puzzling. On one hand, graphene appears to be a strictly 2D material and exhibits such a high crystal quality that electrons can travel submicron distances without scattering. On the other hand, perfect 2D crystals cannot exist in the free state, according to both theory and experiment. This is often reconciled by the fact that all graphene structures studied so far were an integral part of larger 3D structures, either supported by a bulk substrate or embedded in a 3D matrix. We describe individual graphene sheets freely suspended on a microfabricated scaffold. These membranes are only one atom thick and still display a long-range crystalline order. However, our studies by transmission electron microscopy have revealed that suspended graphene sheets are not perfectly flat but exhibit intrinsic microscopic roughening such that the surface normal varies by several degrees and out-of-plane deformations reach 1 nm. The atomically-thin single-crystal membranes offer an ample scope for fundamental research and new technologies whereas the observed corrugations in the third dimension may shed light on subtle reasons behind the stability of 2D crystals.
8:24AM U28.00003 Electrostatic Deposition of Graphene , ANTON SIDOROV, ElectroOptics Research Institute and Nanotechnology Center, University of Louisville, GAMINI SUMANASEKERA, Department of Physics, University of Louisville, MEHDI YAZDANPAHAN, ElectroOptics Research Institute and Nanotechnology Center, University of Louisville, ROMANEH JALILIAN, P. OUSEPH, Department of Physics, University of Louisville, ROBERT COHN, ElectroOptics Research Institute and Nanotechnology Center, University of Louisville — Loose graphene sheets, one to a few atomic layers thick are often observed on freshly cleaved HOPG surfaces. A simple and reliable technique using electrostatic attraction is demonstrated to transfer these graphene sheets to a selected substrate. Sheets from one to 22 layers thick have been transferred by this method. One sheet after initial deposition is measured by atomic force microscopy to be only atomic layer thick (∼0.35 nm). A few weeks later, this height is seen to increase to ∼0.8 nm. Raman spectroscopy of a single layer shows the emergence of an intense D band which dramatically decreases as the number of layers in the sheet increase. The intense D band in monolayer graphene is attributed to the graphene conforming to the roughness of the substrate.

3Corresponding Author

8:36AM U28.00004 Characterization and Patterning of Ultrathin Epitaxial Graphene Grown on 4H-SiC , XUEBIN LI, ZHIMIN SONG, MICHAEL SPRINKLE, XIAOSONG WU, CLAIRE BERGER, WALTER DE HEER, Georgia Institute of Technology — Ultrathin graphene films are grown on the C face (000-1) of insulating single crystal 4H-SiC substrates by high temperature thermal decomposition of SiC. The films are characterized extensively. Atomic force microscopy images show extended atomically flat micron size terraces. Magneto-transport measurements indicate that transport of the films is dominated by the interface graphene layer which is electron-doped due to the built-in electric field at the interface. The films can be patterned with conventional lithography techniques and ribbons with widths less than 10nm can be produced. We present experimental results on several patterned gated structures.

8:48AM U28.00005 ABSTRACT HAS BEEN MOVED TO P27.00015 –

9:00AM U28.00006 Structural and mechanical properties of ‘graphene oxide’-based paper , DMITRY A. DIKIN, ERIC J. ZIMNEY, SASHA STANKOVICH, RICHARD D. PINER, GEOFFREY H. B. DOMMETT, RODNEY S. RUOFF, Northwestern University, Evanston, IL — Free standing membranes (GO paper) were produced by exfoliation of graphene oxide in water to individual ‘graphene oxide’ sheets (as a colloidal suspension) followed by their re-assembly by vacuum filtration. Study of the structure and morphology of the GO paper revealed that it is composed of highly packed and ordered layers of graphene oxide sheets separated by water molecules. Measurements of the mechanical response under tensile load revealed elastic deformation for small strain, followed by plastic deformation again for a relatively small region of strain, and then fracture without pullout of individual graphene oxide layers or multiple cracks. GO paper possesses high modulus values of about 100 GPa, and high strength values around 130 MPa; each much higher than modulus or strength values for Bucky-paper or Grafoil. The experimental results support the conclusions of very effective load distribution and good binding between the GO sheets in which the self-adjusted amount of interlayer water plays a central role. After the deoxygenation of GO sheets the fabricated paper becomes a tunable semiconductor. Support from NASA (Award #: NCC-1-2037) through the University Research, Engineering, and Technology Institute on Bio-inspired Materials is appreciated.

9:12AM U28.00007 Generation of Carbon Scrolls from Graphene films , HUMBERTO GUTIERREZ, AWNISH GUPTA, QIUJIE LU, VINCENT CRESPI, PETER EKLUND, Department of Physics, Pennsylvania State University — Using a chemical process to delaminate graphene from HOPG, we are able to produce suspended graphene and n-graphene layer films (i.e., nGLs, n=integer) in various organic solvents. The nGLs have lateral dimensions of several microns. We observe that in a matter of a few hours, the nGLs “roll up” on themselves to form scrolls. Here we present results of a study which investigates the role of the solvent in determining the characteristic time to “roll up” the nGL. Raman scattering, AFM and TEM is used to characterize the scrolls. A model will be presented to explain why the scrolling occurs.

9:24AM U28.00008 Mechanism of growth of a graphitic edge in a Carbon Monoxide atmosphere , SUJATA PAUL, ERIK E. SANTISO, MARCO B. NARDELLI, NC State University, Raleigh, NC — The interaction of CO with zigzag and armchair graphite edge has been studied using density functional theory. Our results suggest that the growth of a zigzag graphene edge in a CO atmosphere may happen through a multiple steps. A possible growth mechanism will start through the formation of pentagon with the adsorption of CO on the edge. The cleaning of oxygen atoms from the edge could happen through the desorption of CO2 or desorption of O2. Further chemisorption of CO will cover the edge with the formation of 5-7-5 structures. Such adsorptions of CO will be followed by desorption of O2 or desorption of CO2 and finally through the rearrangement of the 5-7-5 structures, the zigzag edge would be restored. On the contrary the growth of armchair graphite edge have only two steps. The formation of hexagonal structures upon adsorption of CO and desorption of top oxygen atoms as CO2 or O2 . Our results of energy calculations suggest that the growth in the direction of a armchair wall is more favorable.

9:36AM U28.00009 Boron doped graphene nanoribbons , THIAGO MARTINS, Instituto de Física - Universidade de Sao Paulo, HIROKI MIWA, Instituto de Física, Universidade Federal de Uberlândia, ANTONIO J.R. DA SILVA, A. FAZZIO, Instituto de Física - Universidade de Sao Paulo — We will present a detailed study of the electronic, magnetic and transport properties of boron doped graphene nanoribbons, for various widths. The electronic structures and the equilibrium geometries were obtained through ab initio total energy DFT calculations. The transport properties were investigated using nonequilibrium Green’s functions. Our results reveal that the substitutional boron atoms occupy the edge sites of nanoribbons, quenching the local ferromagnetism along the nanoribbon edges. In addition, the presence of edge boron atoms break the symmetry between spin up and spin down transmission channels. Those results suggest that, through a suitable doping process, it is possible to tailor the electronic current along the graphene nanoribbon. We thank FAPESP, CNPq and CENAPAD-SP.

9:48AM U28.00010 Thermal-closing of holes put in single-graphene sheets of carbon nanotubes depending on its curvatures , MASAKO YUDASAKA, NEC Corporation, JIN MIYAWAKI, Japan Science and Technology Agency (JST), RYOTA YUGE, TAKASUMI KAWAI, NEC Corporation, JING FAN, JST, SUMIO IJIMA, Meijo University — Holes put in the walls of single-wall carbon nanotubes by oxidation are believed to be closed by heat treatment. We investigated this in detail using single-wall carbon nanohorn (SWNH), a type of single-wall carbon nanotubes. SWNHs are suitable to study this because they have high purities (95%, no metal) and closed structure in the as-grown state, and the holes are easily opened by oxidation. Even numbers and sizes of holes are controllable. The nitrogen adsorption quantities measured at 77K clarified that the holes opened at the tips of tubes were closed easily by heat treatment at 1473K in Ar, but those in the sidewalls were not, suggesting that the closing easiness depended on the tube curvatures. This was confirmed by the computer simulation. The hole closing kinetics of the tip holes was further investigated by changing the heat-treatment duration, as a result, two types of holes were found: one closed in a couple of minutes and the other in 30 minutes by the heat-treatment a 1473K, which may correspond to the variation of hole-sizes at the tips.

10:00AM U28.00011 Fabrication of graphene nanogaps by electrical breakdown , BRIAN STANDLEY, EMMA SCHMIDGALL, MARC BOCKRATH, California Institute of Technology — We have fabricated n-graphene nanogaps which may be useful as an alternative to the metallic contacts used in current single molecule sensors. The nanogaps are formed by electrical breakdown of two-terminal n-graphene devices. We have characterized the gaps by atomic force microscopy and electrical transport measurements, both of which suggest that the gaps are narrow enough to capture a single molecule. The n-graphene contacts’ two dimensional nature is expected to improve gate control by reducing charge screening. Additionally, the contacts’ atomic flatness may allow in situ scanning tunneling microscopy imaging of the transistor molecule.
10:12AM U28.00012 Structural Differences Between Graphite Grown on Si- and C-Terminated Polar Faces of 4H-SiC\textsuperscript{1}. JOANNA HASS, RUI FENG, XUEBIN LI, MICHAEL SPRINKLE, Georgia Institute of Technology, CLAIRE BERGER, CNRS-LEPES, EDWARD CONRAD, Georgia Institute of Technology — In the last two years the transport properties of 2D graphene grown on SiC have shown that electron coherence lengths can exceed many microns. It is now critical to understand the source of these unique transport properties and explain their dependence on which polar face they are grown. We will present surface X-ray diffraction data that highlights the structural differences between graphite grown on C-terminated and Si-terminated 4H-SiC. We will show that the C-terminated graphite grows in domains more than an order of magnitude larger than the Si-terminated graphite.\textsuperscript{1} Strain, islanding and complex rotational phases in the graphite will be presented. More importantly, X-ray reflectivity measurements reveal a tightly bound initial graphene layer, with a second graphene layer at an interlayer spacing significantly larger than in the bulk. The implications of this “buffer” layer will be discussed in terms of recent band structure calculations\textsuperscript{2} and a possible explanation for transport seemingly confined to a single graphene layer. \textsuperscript{1} J. Hass, et al., App. Phys. Lett. 89, 143106 (2006). \textsuperscript{2} F. Varchon, et al., (to be published).

\textsuperscript{1} NSF, Intel Corp.

10:24AM U28.00013 Graphane: a two-dimensional hydrocarbon, JORGE SOFO, AJAY CHAUDHARI, GREG BARBER, Penn State — We predict the stability of a new extended two-dimensional hydrocarbon on the basis of first-principles total energy calculations. The compound that we call graphane is a fully saturated hydrocarbon derived from a single graphene sheet with formula CH. All of the carbon atoms are in sp\textsuperscript{3} hybridization forming a hexagonal network and the hydrogen atoms are bonded to carbon on both sides of the plane in an alternating manner. Graphane is predicted to be stable with a binding energy comparable to other hydrocarbons such as benzene, cyclohexane, and polyethylene. We discuss possible routes for synthesizing graphane and potential applications as a hydrogen storage material and in two dimensional electronics.

10:36AM U28.00014 Morphology and crack toughness behaviour of PP-MWNT nanocomposites, R. WEIDISCH, M. GANSS, B. K. SATAPATHY, Institute of Material Science and Technology, Friedrich Schiller University-Jena, Germany, P. POETSCHEKE, D. JEHNICHEN, A. JANKE, Leibniz Institute of Polymer Research, Dresden, Germany — Morphology and crack toughness of PP-MWNT nanocomposites have been studied by AFM-WAXD and essential work of fracture approach respectively. A ductile-to-semi-ductile transition in the crack resistance behaviour of PP-MWNT nanocomposites and its interrelation to the structural attributes studied by SEM and DSC has been discussed. A maximum in the non-essential work of fracture was observed at 0.5 wt.-% MWNT demonstrating enhanced toughness compared to pure PP, followed by a sharp decline as the MWNT content was increased to 1.5 wt.-% reveals a ductile-to-semi-ductile transition. Fracture kinetics studies presents a qualitative picture of the nature of such a transition in terms of (a) switch over from non-steady (in pure PP) to steady state crack-tip-opening-displacement rate (in nanocomposites) and (b) ductile-to-semi-ductile transition being largely due to delayed-yielding in the nanocomposites. The time-resolved analysis of strain field offering insight into the crack propagation kinetics has revealed that such a transition is caused by rapid development of critical local stresses causing a shift of crack initiation to shorter time, resulting in a semi-ductile fracture of nanocomposites containing 1.5 wt.-% MWNT.

10:48AM U28.00015 Electron fractionalization in two-dimensional graphene-like structures\textsuperscript{1}. CHANG-YU HOU, CLAUDIO CHAMON, Department of Physics, Boston University, CHRISTOPHER MUDRY, Condensed matter theory group, Paul Scherrer Institut, Switzerland — Electron fractionalization is intimately related to topology. In one-dimensional systems, fractionally charged states exist at domain walls between degenerate vacua. In two-dimensional systems, fractionalization exists in quantum Hall fluids, where time-reversal symmetry is broken by a large external magnetic field. Recently, there has been a tremendous effort in the search for examples of fractionalization in two-dimensional systems with time-reversal symmetry. In this paper, we show that fractionally charged topological excitations exist on graphene-like structures, where quasiparticles are described by two flavors of Dirac fermions and time-reversal symmetry is respected. The topological zero-modes are mathematically similar to fractional vortices in j-wave superconductors. They correspond to a twist in the phase in the mass of the Dirac fermions, akin to cosmic strings in particle physics.

\textsuperscript{1} NSF grant DMR-0305482 (C.-Y. H and C. C.).

Thursday, March 8, 2007 8:00AM - 10:36AM — Session U44 DMP: Focus Session: Optical Properties of Metallic Nanostructures: Theory

8:00AM U44.00001 Theory and modeling of light interactions with metallic nanostructures\textsuperscript{1}, STEPHEN GRAY, Argonne National Laboratory — Metallic nanostructures such as systems containing metal nanoparticles or metal films with nanoscale diameter holes or other nanostructured features are intriguing systems. Surface plasmons, special electronic excitations near the metallic surfaces, can then be excited with visible light. In addition to interest in their fundamental behavior and interactions, surface plasmons are useful in a variety of practical areas, including chemical and biological sensing and optoelectronics. Surface plasmons can be intense and localized, and correctly describing their behavior in complex systems can require numerically rigorous modeling techniques. This talk presents a discussion of the results of rigorous electrodynamics modeling using the finite-difference time-domain (FDTD) method. Such calculations may be used to validate ideas and concepts based on approximate models. Detailed inspection and analysis of the results can also lead to the development of new physical pictures. In particular, FDTD calculations are used to show (i) how it is possible to design systems that can achieve high directive radiation, (ii) how nanoholes and wells in metal films can exhibit complex transmission spectra of relevance to sensing, and (iii) how nanoholes and wells in metal films can exhibit complex transmission spectra of relevance to sensing.

\textsuperscript{1} Argonne National Laboratory’s work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences under contract DE-AC02-06CH11357.

8:36AM U44.00002 General Properties of Local Plasmons in Metal Nanostructures\textsuperscript{1}, FENG WANG, RON SHEN, UC Berkeley and Materials Science Division, LBNL — Local plasmon resonance in metal nanostructures offers the potential to concentrate electro-magnetic energies at nanoscale. Different designs of nanostructures have been proposed to achieve this goal. Here we investigate the general behavior of local plasmon resonances independent of specific structures. We study the local plasmon under quasi-static approximation given that nanostructure dimension is much smaller than optical wavelength.\textsuperscript{1} We show that the plasmon resonance frequency depends on the fraction of plasmon energy residing in the metal through the real dielectric function of the metal. Further, at a given resonant frequency, the Q-factor of the resonance is determined only by the complex dielectric function of the metal material and does not depend on the nanostructure form or the dielectric environment. We will also discuss the effect of optical gain on the Q-factor of plasmon resonance.

\textsuperscript{1}This work was supported by the Miller Institute of the University of California at Berkeley and the Department of energy.
nanoshells provides a new and efficient method for identifying these versatile nanostructures and for studying their mechanical and structural properties. Of the nanoshell surface plasmon resonance. The modulation amplitude is significantly stronger while the period is longer than in a gold nanoparticle of the same

BAZYAN, Jackson State University, C. GUILLON, P. LANGOT, N. DEL FATTI, F. VALLEE, Centre de Physique Moleculaire Optique et Hertzienne CNRS and Enhanced Infrared Absorption (SEIRA) applications. The efficiency of the close-packed array is around three orders of magnitude higher than that for an individual nanoshell. The largest efficiencies occur for incident enhancements of the nanoshell array is a factor of 10 higher than that of an individual nanoshell. The calculated Surface Enhanced Raman Spectroscopy (SERS) calculated extinction spectrum agrees very well with experimental data. We show that compared with an individual nanoshell or a nanoshell trimer, the nanoshell method to calculate the optical properties of a two dimensional close-packed array of gold nanoshells for different polarizations under normal incidence. The

WANG, NAOMI HALAS, PETER NORDLANDER, Rice University — Using periodic boundary conditions, we employ the Finite Difference Time Domain (FDTD) method, we calculate the near- and far-field properties of a gold nanostar. The nanostar is modeled as a solid core with protruding tips of prolate spheroidal shape. The shape of this nanostar agrees qualitatively with the shape inferred from an SEM picture. The calculated extinction spectra agree very well with the experimentally observed scattering spectra for different polarization angles of incident light. We show that the plasmon resonances of the nanostar can be viewed as resulting from hybridization of short wavelength primitive plasmons associated with the core and long wavelengths plasmons associated with the individual tips. Due to the asymmetric orientation of the tips, several nanostars plasmons can be observed for an arbitrary polarization of the incident light. The intensity of these plasmons resonances vary with polarization angle. The plasmon hybridization results in bonding and antibonding nanostar plasmons. The bonding plasmons of this nanostar agrees qualitatively with the shape inferred from an SEM picture. The calculated extinction spectra agree very well with the experimentally observed scattering spectra for different polarization angles of incident light. We show that the plasmon resonances of the nanostar can be viewed as resulting from hybridization of short wavelength primitive plasmons associated with the core and long wavelengths plasmons associated with the individual tips. Due to the asymmetric orientation of the tips, several nanostars plasmons can be observed for an arbitrary polarization of the incident light. The intensity of these plasmons resonances vary with polarization angle. The plasmon hybridization results in bonding and antibonding nanostar plasmons. The bonding plasmons are primarily composed of primitive tip plasmons but with a small but finite admixture of the core plasmons. The admixture of the core plasmon dramatically increases the cross section for excitation of the bonding plasmons and result in enormous local electric field enhancements compared to those for individual tips.

9:36AM U44.00007 FDTD calculations of the optical properties of nanostars, F. HAO, C. NEHL, J. HAFNER, P. NORDLANDER, Department of Physics, Rice University, Houston TX 77251 — Using the Finite-Difference Time-Domain (FDTD) method, we calculate the near- and far-field properties of a gold nanostar. The nanostar is modeled as a solid core with protruding tips of prolate spheroidal shape. The shape of this nanostar agrees qualitatively with the shape inferred from an SEM picture. The calculated extinction spectra agree very well with the experimentally observed scattering spectra for different polarization angles of incident light. We show that the plasmon resonances of the nanostar can be viewed as resulting from hybridization of short wavelength primitive plasmons associated with the core and long wavelengths plasmons associated with the individual tips. Due to the asymmetric orientation of the tips, several nanostars plasmons can be observed for an arbitrary polarization of the incident light. The intensity of these plasmons resonances vary with polarization angle. The plasmon hybridization results in bonding and antibonding nanostar plasmons. The bonding plasmons are primarily composed of primitive tip plasmons but with a small but finite admixture of the core plasmons. The admixture of the core plasmon dramatically increases the cross section for excitation of the bonding plasmons and result in enormous local electric field enhancements compared to those for individual tips.

9:48AM U44.00008 Optical Properties of Semiconducting and Metallic Nanoparticle Structures by TDDFT, EMILY TOWNSEND, GARNETT BRYANT, National Institute of Standards and Technology — Superstructures of semiconducting and metallic nanoparticles display substantially novel properties compared to homogeneous materials or single nanoparticles due to the coupling of elementary excitations between different nanoparticles, i.e. the confined plasmons in the metallic nanoparticles and excitons in semiconductor quantum dots. We use time-dependent density functional theory (TDDFT) to examine the optical response of such structures. This method allows a quantitative, fully quantum mechanical treatment of the electronic response of both the semiconducting and metallic components.

10:00AM U44.00009 Optical Properties of 2D hexagonal arrays of gold nanoshells, FEI LE, HUI WANG, NAOMI HALAS, PETER NORDLANDER, Rice University — Using periodic boundary conditions, we employ the Finite Difference Time Domain method to calculate the optical properties of a two dimensional close-packed array of gold nanoshells for different polarizations under normal incidence. The calculated extinction spectrum agrees very well with experimental data. We show that compared with an individual nanoshell or a nanoshell trimer, the nanoshell array shows a significantly red shifted dipolar resonance while the quadrupolar peak remains at almost the same wavelength for all structures. The local field enhancement of the nanoshell array is a factor of 10 higher than that of an individual nanoshell. The calculated Surface Enhanced Raman Spectroscopy (SERS) efficiency of the close-packed array is around three orders of magnitude higher than that for an individual nanoshell. The largest efficiencies occur for incident wavelengths around six microns in the infrared. The 2D hexagonal array of gold nanoshells is therefore highly suitable as a substrate for both SERS and Surface Enhanced Infrared Absorption (SEIRA) applications.

10:12AM U44.00010 Coherent acoustic vibrations of metal nanoshells, A.S. KIRAKOSYAN, T.V. SHAH-BAZYAN, Jackson State University, C. GUILLON, P. LANGOT, N. DEL FATTI, F. VALLEE, Centre de Physique Moleculaire Optique et Hertzienne CNRS and Universite Bordeaux I, France, T. CARDINAL, M. TREGUER, Institut de Chimie de la Matiere Condensee de Bordeaux CNRS and Universite Bordeaux I, France — We study vibrational modes of gold nanoshells grown on dielectric core by means of time-resolved pump-probe spectroscopy. The fundamental breathing mode launched by a femtosecond pump pulse manifests itself in a pronounced time-domain modulation of the differential transmission probed at the frequency of the nanoshell surface plasmon resonance. The modulation amplitude is significantly stronger while the period is longer than in a gold nanoparticle of the same overall size. A theoretical model describing breathing mode frequency and damping for a nanoshell in a medium is developed. A distinct acoustical signature of nanoshells provides a new and efficient method for identifying these versatile nanostructures and for studying their mechanical and structural properties.
10:24AM U44.00011 Surface plasmon polaritons in co-metal nanostructures,1 KRZYSZTOF KEMP, Boston College — Co-metal structures, such as a strip-line or coaxial cable, are well-known from radio engineering. They are capable of subwavelength guiding of TEM modes, and therefore their visible range analogs are of great interest. At these very high frequencies, however, the propagating modes acquire a plasmon polariton character. I study in detail these plasmon polaritons in co-metal nanostructures, and show that for properly chosen materials and geometry, these modes reduce to the conventional, radio TEM modes. I show, how a metamedium made of an array of such co-metal nanostructures, can simulate negative refraction, suerlensing and cloaking.

1This work was supported by the Massachusetts Technology Transfer Center (2005 Technology Investigation Award).

Thursday, March 8, 2007 11:15AM - 1:39PM Session V11 DMP: Heavy Fermions Colorado Convention Center Korbel 1F

11:15AM V11.00001 Magnetic Field Effects in the Heavy Fermion Ce3Co4Sn13, A.D. CHRISTIANSON, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, F. RONNING, Y. TOKIWA, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, J.S. GARDNER, H.J. KANG, J.H. CHUNG, NIST Center for Neutron Research, Gaithersburg, Maryland 20899, USA, E.A. GOREMYCHKIN, P. MANUEL, Rutherford Appleton Laboratory, Chilton, Didcot OX11 0QX, United Kingdom, J.D. THOMPSON, J.L. SARRAO, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, A.L. CORNELIUS, University of Nevada, Las Vegas, 89154, USA, J.M. LAWRENCE, University of California, Irvine, California 92697, USA — Ce3Co4Sn13 is a heavy Fermion system with a low temperature specific heat as large as 4 J/mol K2. Measurements on single crystal specimens of the elastic neutron scattering response and the heat capacity (C) show that Ce3Co4Sn13 is extremely sensitive to applied magnetic fields. The heat capacity measurements show that the broad peak in C/T at 0.8 K at zero field initially moves downward in temperature before moving upward with a characteristic energy scale of 2 T. Neutron diffraction measurements at 0.15 K show that upon application of very small magnetic fields, the intensity on the (100) peak grows and does not saturate below 6 T. Although reduced in magnitude the effect persists to temperatures as high as 2 K.

11:27AM V11.00002 Thermal Expansion of the Heavy Fermion Borocarbide YbNi3B2C, G.M. SCHMIEDEHOFF, A.W. LOUNSBY, D.J. LUNA, W.E. OKRAKU, S.J. TRACY, J.C. COOLEY, S.L. BUD'KO, P.C. CANFIELD, Occidental College — YbNi3B2C is a heavy fermion compound with a coherence temperature of about 10 K. We have measured its thermal expansion from room temperature to below 1 K. The thermal expansion is anisotropic, negative below about 16 K, and deviates from simple metallic behavior near the coherence temperature. We will present and discuss our results in the context of a Gruneisen analysis. This work was supported by the National Science Foundation under DMR-0305397. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-ENG-82. This work was supported by the Director for Energy Research, Office of Basic Energy Sciences.

11:39AM V11.00003 Infrared and magneto-optical studies of heavy fermion skutterudites YbFe12Sb12 and CeRu12Sb12, L.W. KOHLMAN, S.V. DORDEVIC, The University of Akron, K.S.D. BEACH, Boston University, D.N. BASOV, R. BAUMBACH, M.B. MAPLE, University of California, San Diego, R. TUNG, Y.J. WANG, National High Magnetic Field Lab, N. TAKEDA, University of Tokyo, Japan — We will report infrared and magneto-optical results on two heavy fermion skutterudites YbFe12Sb12 and CeRu12Sb12. Detailed temperature dependence of infrared spectra will be presented for both compounds. In addition, magneto-transmission measurements on YbFe12Sb12 in magnetic field as high as 33 Tesla, and magneto-reflection measurements on CeRu12Sb12 in 17 Tesla field will be reported. The results reveal suppression of heavy fermion state with magnetic field, and recovery of a more conventional metallic state. In particular, the effective mass of charge carriers is gradually diminished. On the other hand, hybridization gap is much more insensitive to the application of magnetic field.

11:51AM V11.00004 Kondo ground state of 6 related Yb-based intermetallic compounds, E.D. MUN, S. JIA, Ames Laboratory, Dept of Physics and Astronomy, Iowa State University, M.S. TORIKACHVILI, Dept. of Physics, San Diego State University, A.S. SEFAT, S.L. BUD’KO, P.C. CANFIELD, Ames Laboratory, Dept of Physics and Astronomy, Iowa State University — Isostructural YbT2Zn20 (T=Fe, Co, Ru, Rh, Os, Ir) have less than 5% concentration atomic Yb, in which the Yb atoms fully occupy one unique crystallographic site of cubic (-43m) symmetry. This series of compounds offer the opportunity to systematically study Kondo lattice systems approaching the single ion limit. With the thermodynamic and transport measurements, we show that the Kondo ground state has different degeneracies for T=Fe, Ru, Rh, Os and Ir, reflecting the competition between the different Kondo temperatures (TK) and the similar crystal-electric field (CEF) splitting temperatures (TCEF). On the other hand, the unusual thermodynamic behavior at low temperature suggests that YbCo2Zn20 has low TK and seems to be very close to a quantum critical point.

12:03PM V11.00005 Spin Dynamics in the f-electron non Fermi liquid alloy Sc1-xUpxPd3, STEPHEN WILSON, University of Tennessee, PENCHENG DAI, University of Tennessee/ Oak Ridge National Laboratory, D. ADROJA, ISIS Rutherford Appleton Laboratory, Y. QIU, NIST Center for Neutron Research, N.P. BUTCH, M.B. MAPLE, University of California, San Diego — We will discuss our recent inelastic neutron scattering experiments probing the spin dynamics in the non Fermi-liquid alloy, Sc1−xUpxPd3. The increased homogeneity of U- sites in this system allows for an investigation of magnetism without the disordering effects of U-site clustering observed in isostructural Y1−xUxPd3. Spin dynamics indicative of the influence of a spin glass (SG) quantum critical point (QCP) in Sc1−xUxPd3 have been observed previously. Our current study probes spin fluctuations now doped away from this SG QCP and into the antiferromagnetic (AF) ordered phase of the system. The evolution of the spin excitations as the system is tuned across its phase diagram away from the SG QCP will be discussed, with particular emphasis to the evolution of the localized spin fluctuations attributed to the QCP in this system.

12:15PM V11.00006 Interplay between Disorder and Quantum and Thermal Fluctuations in Ferromagnetic Alloys — New Systems1 G.R. STEWART, J.S. KIM, University of Florida, M.B. SILVA NETO, ITP, University of Stuttgart, A.H. CASTRO NETO, Boston University — Previously1 we addressed the effects of disorder on the ferromagnetic ordering temperature, TC, in UCuSi2−xGe2. In that work the measured non-monicotonic variation of TC with disorder (as measured by the resistivity) could be explained within a model2 of localized spins interacting with an electronic bath. This model predicts that, in some cases, TC can be enhanced by the interplay between quantum and thermal fluctuations with disorder. We have extended this work to other ferromagnetic alloys, with both significantly larger as well as similar variations of TC with doping compared to the ~10 % variation of TC observed in UCuSi2−xGe2. Resistivity, magnetic susceptibility, and specific heat will be presented, along with a comparison to the theory2. 1M. B. Silva Neto, A. H. Castro Neto, D. Mixon, J. S. Kim, and G. R. Stewart, Phys. Rev. Lett. 91, 257206 (2003). 2M. B. Silva Neto and A. H. Castro Neto, Europhys. Lett. 62, 890 (2003).

1Work at UF supported by DOE contract no. DE-FG02-86ER45268; work at BU supported by NSF contract no. DMR-0343790.
12:27PM V11.00007 Effects of Disorder in the Heavy Fermion Antiferromagnet CeCu$_{6-x}$Au$_x$. D.I. BURNETTE, J.S. KIM, G.R. STEWART, University of Florida — Using a quick quenching technique that also produces bars of known geometry for absolute resistivity measurements, we have measured the effects of this fairly rapid ($\sim 10^4$ K/s) solidification on the high angle x-ray line width, resistivity, magnetic susceptibility, and specific heat of CeCu$_{6-x}$Au$_x$ for several compositions. Gradual variations of the disorder and its effect on the properties were investigated by annealing the quenched samples at 700 °C over periods of days to weeks. The discussion of the effects of the quenched-in disorder on the measured properties will focus on $T_C(x)$, the low temperature specific heat $\gamma$, and the non-Fermi liquid behavior.

3Work at Florida supported under DOE contract no. DE-FG02-86ER45268.

12:39PM V11.00008 Elastic property of a high-field ordered state observed in PrFe$_2$P$_{12}$, YOSHIKI NAKANISHI, TAKUYA FUJINO, PELIEE SUN, MITSUTERU NAKAMURA, MASAHITO YOSHIZAWA, Iwate Univ., HITOSHI SUGAWARA, Tokushima Univ., DAISUKE KIKUCHI, HIDEYUKI SATO, Tokyo Metropolitan Univ. — We present experimental results of elastic constants as a function of temperature and magnetic field for the Pr-based heavy fermion system PrFe$_2$P$_{12}$, especially in a high-field (HF) ordered phase discovered. Since the HF phase exists in a narrow temperature range below 0.7 K and for high fields above 7 T in a highly limited angular range around the [111] directions, the elastic constants $C_L = (C_{11}+2C_{12}+4C_{44})/3$ and $C_T = (C_{11}-C_{12}+C_{44})/3$ were measured by the longitudinal (L) one propagating along the [111] direction and by the transverse (T) one along the [111] direction polarized to the [1-11] one, respectively. A clear upturn was observed in both of the elastic constants below the HF ordered phase transition temperature. Furthermore, a remarkable elastic softening toward the transition temperature was observed in the temperature dependence of $C_{11}$, whereas no softening was observed in $C_T$. These results indicate that the softening is most likely to be due to the bulk modulus ($C_{11}+2C_{12}$). Thus, it is expected that the HF ordered phase seems to be accompanied by a strain fluctuation with a multi-polar moment is a candidate for the HF ordered phase.

12:51PM V11.00009 Disorder and quantum size effects on Kondo interactions and magnetic correlation in CePt$_2$. Y.Y. CHEN, T.K. LEE, Institute of Physics, Academia Sinica, Taipei, Taiwan, J.M. LAWRENCE, Department of Physics and Astronomy, University of California, Irvine, California, C.H. BOOTH, Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California — Measurements of specific heat $C(T)$ and magnetic susceptibility $\chi(T)$ on a series of CePt$_2$ nanoparticles with size $d = 3.1$, 22 and 26 nm are compared to those of bulk CePt$_2$ to determine the size effects on Kondo interactions and magnetic correlation therein. Kondo interactions ($T_K = 5.6$ K) and an antiferromagnetic correlation ($T_N = 1.6$ K) coexist in CePt$_2$ with ~60% and ~40% of Ce magnetic ions involved in respective. While the antiferromagnetism is diminished by size reduction, Kondo behaviour predominates, with a sommerfield constant $\gamma$ increasing from 460 mJ/f.u. K$^2$ for the bulk to 3000 mJ/f.u. K$^2$ for 3.1 nm. Meanwhile, a decrease of Kondo temperature $T_K$ from 5.6 to 0.42 K is observed with the size reduction. The consequences were explained by structural disorders, however for $d < 10$ nm electronic quantum size effect play a more significant role.

1:03PM V11.00010 Probing the Magnetic Order of UPT$_3$ by Magnetoresistance. THOMAS M. LIPPMAN, JOHN P. DAVIS, HYOUNGSOON CHOI, JOHANNES POLLANEN, WILLIAM J. GANNON, WILLIAM P. HALPERIN, Northwestern University — It is believed that magnetic order has a strong influence on the unconventional superconducting state of UP$_3$. Measurements of specific heat $C(T)$ and magnetic susceptibility $\chi(T) on a series of CePt$_2$ nanoparticles with size $d = 3.1$, 22 and 26 nm are compared to those of bulk CePt$_2$ to determine the size effects on Kondo interactions and magnetic correlation therein. Kondo interactions ($T_K = 5.6$ K) and an antiferromagnetic correlation ($T_N = 1.6$ K) coexist in CePt$_2$ with ~60% and ~40% of Ce magnetic ions involved in respective. While the antiferromagnetism is diminished by size reduction, Kondo behaviour predominates, with a sommerfield constant $\gamma$ increasing from 460 mJ/f.u. K$^2$ for the bulk to 3000 mJ/f.u. K$^2$ for 3.1 nm. Meanwhile, a decrease of Kondo temperature $T_K$ from 5.6 to 0.42 K is observed with the size reduction. The consequences were explained by structural disorders, however for $d < 10$ nm electronic quantum size effect play a more significant role.

1:15PM V11.00011 Doped Mott insulator physics in the 4f antiferromagnet CeIn3 and implications for pressure-tuned superconductivity. NEIL HARRISON, Los Alamos National Labs, SUCHITRA SEBASTIAN, Cavendish Lab, CRISTIAN BATISTA, MARCELO JAIME, STUART TRUGMANN, VICTOR FANELLI, Los Alamos National Labs, TAKAO EBHIARA, Shizuoka Univ., ERIC PALM, TIM MURPHY, Florida State Univ., HISATOMO HARIMA, Kobe Univ. — We report recent de Haas–van Alphen experiments performed at low temperatures ($T > 30$ mK) and high magnetic fields in CeIn$_3$ that motivate us to revise our understanding of strongly coupled antiferromagnetism in f-electron systems. In addition to the known light Fermi surface sheets, heavy ellipsoid pockets are observed with a symmetry consistent with them being situated at the $\pi/2, \pi/2, \pi/2$ point in the paramagnetic Brillouin zone. Their topology is the 3D analog of the 2D hole pockets reported to exist at $\pi/2, \pi/2$ in underdoped cuprate superconductors, indicating some degree of similarity between the electronic structures in the d- and f-electron systems. The effective masses of the ellipsoids are sufficient for all of the electronic specific heat of CeIn$_3$, at ambient pressure within the antiferromagnetic phase, making them strong candidates for the origin of the coexisting superconductivity under pressure. High magnetic fields cause these pockets to undergo a topological deformation, passing through a Lifshitz transition at $\sim 40$ T.

1:27PM V11.00012 The superconducting pairing states in CeCu$_2$Si$_2$. H. Q. YUAN, M. B. SALAMON, University of Illinois at Urbana and Champaign, H. S. JEEVAN, C. GEIBEL, F. STEGLICH, Max-Planck-Institute for Chemical Physics of Solids — The prototype heavy fermion superconductor CeCu$_2$Si$_2$ exhibits very rich physical properties. It has been shown that two distinct superconducting states, one around an AFM QCP at low pressures and the other one around a weak-first order valence transition at high pressures, uniquely exist in the pressurized CeCu$_2$(Si/Ge)$_2$ [1]. In this talk, I will first briefly review the recent progress on the study of these two superconducting phases. Then I will focus on the superconducting pairing state of CeCu$_2$Si$_2$ at $p = 0$. Early measurements, e.g., specific heat and $\mu$SR, revealed quite controversial behavior due to the limitations of experimental techniques and sample quality. In order to elucidate the nature of superconductivity in CeCu$_2$Si$_2$ and to investigate the interplay of AFM and superconductivity, we performed precise measurements of the magnetic penetration depth $\Delta\lambda(T)$ in high quality single crystals down to $T = 80$ mK. A linear temperature dependence of $\lambda(T)$ is observed in both A/S-type and S-type CeCu$_2$Si$_2$ below $T = 150$ mK, providing uncontroversial evidence for the existence of line nodes in the superconducting energy gap. [1] H. Q. Yuan et al., Science 302, 2104 (2003); Phys. Rev. Lett. 96, 047008 (2006).

Thursday, March 8, 2007 11:15AM - 2:15PM —
Session V12 GMAG DMP FLAP: Focus session: Magneto-optics and Spin Dynamics
Colorado Convention Center Korbel 3C
11:15 AM V12.00001 Determination of effective sp-d exchange integrals in wide-gap DMS. 
WOJCIECH PACUSKI, University Grenoble 1 and Warsaw University — This work presents a magneto-optical study of diluted magnetic semiconductors (DMS) based on ZnO and GaN and doped with manganese, iron, and cobalt. Both host materials, ZnO and GaN, are wide bandgap semiconductors with a wurtzite structure, a weak spin-orbit coupling and a strong electron-hole exchange interaction within the excitons. In the presence of magnetic field, the magnetic ions induce in such materials giant Zeeman effect with no straightforward interpretation, e.g.: excitons anti-cross, and not only the transition energies, but also the oscillator strengths are strongly affected by the giant Zeeman effect. On thin epitaxial layers grown on (0001) sapphire, we observed the giant Zeeman splitting of A and B excitons which are optically active in the Faraday configuration when the propagating light is parallel to the c-axis. The Zeeman splitting decreases with the temperature and increases non-linearly with the magnetic field, demonstrating a dependence on the magnetization of the localized spins. A quantitative analysis allows us to discuss the detailed behavior of the magnetization and to estimate the p-d exchange integral J for the studied wide bandgap DMS. For the d0 electronic configuration (Mn2+ and Fe3+) the magnetization follows a Brillouin function B0.2, whereas, for d5 or d3 of Co2+ and Mn2+ respectively, the spin orbit coupling and the trigonal crystal field lead to an anisotropic magnetization, consistent with that deduced independently from the analysis of intra-atomic transitions. We find a positive sign of J for GaN:Mn2+ and GaN:Fe3+. Assuming that the valence band ordering in ZnO is Γ5, Γ7, Γ7 (this corresponds to usual, positive sign of the spin-orbit coupling), we find J to be negative for ZnO:Co2+ and ZnO:Mn2+. 


11:51 AM V12.00002 Magneto-optical Kerr Spectroscopy of GaMnAs. C. SUN, D. J. HILTON, J. KONO, Rice University, H. MUNEKATA, Tokyo Institute of Technology, CYWINSKI, L. J. SHAM, University of California San Diego — We have performed static and dynamic magneto-optical Kerr measurements on ferromagnetic GaMnAs as a function of temperature, magnetic field, and photon energy. The static Kerr angle at zero magnetic field, which exists only below the Curie temperature, is a strong function of photon energy in the probed range (1.5-2.5 eV), exhibiting a sign change around 2.35 eV. We will present detailed comparison of the experimental spectra with theoretical spectra calculated based on an 8-band k p model. In two-color ultrafast magneto-optical Kerr measurements, we observe ultrafast demagnetization, similar to what we recently reported for InMnAs [1]. The demagnetization signal (i.e., photoduced decrease in increasing Kerr angle), which decreases with increasing temperature and vanishes at Curie temperature, has two dynamic components: an ultrafast (∼ 1 ps) drop in magnetization is followed by a slower (∼ 100 ps) demagnetization process. The fast component strongly depends on the pump laser fluence. We will discuss how this dynamics changes with the photon energy and polarization of the pump beam, including both above and below band-gap excitation. 1. J. Wang et al., Phys. Rev. Lett. 95, 167401 (2005).

12:03PM V12.00003 Theory of sub-picosecond light-induced demagnetization in GaMnAs and InMnAs. LUKASZ CYWINSKI, L.J. SHAM, University of California, San Diego — When a (III,Mn)V ferromagnetic semiconductor is excited by a strong laser pulse, its magnetization decreases on a sub-picosecond time-scale [1,2]. We explain such rapid magnetization dynamics by spin-flip scattering due to the sp-d exchange interaction between the hot carriers and the localized spins. We derive the equations for the dynamics of Mn spins and phenomenologically describe the energy and spin relaxation of carriers. For efficient demagnetization a large density of states and short spin relaxation time of carriers is necessary, so that the excited holes cause magnetization quenching. The calculation of demagnetization using spin-flip transition rates derived from the 6 band Luttinger model gives results in qualitative agreement with experiments. 1. J. Wang et al., Phys. Rev. Lett. 95, 167401 (2005). 2. J. Wang et al, Phys.: Condens. Matter 18, R501 (2006)

1This work was supported by NSF.

12:15PM V12.00004 Mn ion spin dynamics in GaMnAs quantum wells. R.C. MYERS, M.H. MIKKELSEN, N.P. STERN, A.C. GOSSARD, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — We investigate the spin precession of Mn ions within highly diluted GaMnAs-AlGaAs quantum wells grown by molecular beam epitaxy at intermediate temperature[1]. An exciton bound to the neutral Mn acceptor (A7/2) emits photons at an energy red-shifted from the free exciton emission, thus providing selective optical access to the Mn acceptors within the quantum wells. We observe that the Mn emission can be efficiently oriented using circularly polarized excitation, becoming increasingly efficient for narrow line width excitations close to the exciton absorption edge. In addition, Hanle effect measurements in the quantum wells reveal that the optically-induced polarization of the Mn emission tracks a sharp Lorentzian as a function of magnetic field in the Voigt geometry. We calculate the spin lifetime of the neutral Mn acceptor complex from the width of the Hanle curves and observe an exponential increase in the lifetime with decreasing Mn concentration.

1Work supported by the ONR and NSF.


12:27PM V12.00005 Photo-induced precession of magnetization in ferromagnetic GaMnAs. YUSUKE HASHIMOTO, HIRO MUNEKATA, Imaging Science and Engineering Laboratory, Tokyo Institute of Technology — Precession of magnetization induced by the pure optical excitation with femto-second light pulses has been reported recently through the study of time-resolved magneto-optical (TRMO) signal in ferromagnetic GaMnAs layers [1]. The present work reports newer TRMO data which were obtained very recently with much precise experimental setups and wider time windows. Three different dynamic behaviors have been found in different time windows; (i) a relatively large TRMO oscillation within 300 ps which shows a strong excitation wavelength dependence, (ii) subsequent oscillatory behavior which lasts up to 1 ns with much weaker excitation wavelength dependence, and (iii) rather long TRMO decay signal in 3 ns without spin precession. Temperature and magnetic-field dependences of the signals indicate that these phenomena are associated with ferromagnetism of the sample. The modeling based on Landau-Lifshitz-Gilbert equation with three different magnetization components suggests that a change in magnetic anisotropy occurs immediately after the optical excitation and decays within 100ps, to which magnetization follows with the precessional motion in the sample plane. [1] H. Takechi et al., presented in PASPS-IV (2006); pss-c in print.

12:39PM V12.00006 Time Resolved Magneto-Optical Studies of Ferromagnetic InMnSb Films. MATTHEW FRAZIER, RAJEEV KINI, KANOKWAN NONTAPOT, ALIYA GIFFORD, GITI KHODAPARAST, Department of Physics, Virginia Tech, TOMASZ WOJTOWICZ, Institute of Physics, Polish Academy of Sciences, XINYU LIU, JACEK FURDYNA, Department of Physics, University of Notre Dame — Current research activities in the area of ferromagnetic semiconductor have been mainly focused on III-Mn-V alloys with small lattice constants and large effective masses of valence-band such as GaMnAs. Various theoretical models have been proposed to explain the actual mechanism of ferromagnetism in III-Mn-Vs but the microscopic mechanism is still a matter of controversy. It is therefore important to explore the opposite extreme of the III-Mn-V ternaries i.e., InMnSb, which has the largest lattice constant in this family of materials. We report magneto-optical measurements in time domain of photo-induced spin and carrier in InMnSb and compare them to analogous measurements in InBeSb and InSb films. In this work, magneto-optical Kerr effect and standard pump-probe technique provided a direct measure of the photo-excited spin and carrier lifetimes, respectively. Our measurements provide new information on the dynamics and interactions in these materials systems.

1Supported by: NSF-DMR-0507866, AFOSR Young Investigator Program, Jeffress Trust Fund-J748, Advance-VT, NSF-DMR06-03752.
12:51PM V12.00007 Ultrafast Photo-induced Ferromagnetism in III-Mn-V Semiconductors, INGRID COTOROS, University of California and Lawrence Berkeley National Lab, Berkeley CA 94720, JIGANG WANG, K.M. DANI, Lawrence Berkeley National Lab, Berkeley CA 94720 — We report on ultrafast photoenhancement of hole-mediated ferromagnetism, and paramagnetic to ferromagnetic phase transition in III-Mn-V semiconductor GaMnAs via laser excited transient carriers. Our femtosecond UV pump/NIR probe vectorial MOC spectroscopy reveals sub-picosecond demagnetization, precessional trajectory of the magnetization vector, and establishment of the ferromagnetic order on a 100-ps time scale. The dynamic enhancement of the magnetic ordering, manifesting as the photo-induced magnetization below and above the Curie temperature $T_c$, is well explained by a transient increase of $T_c$ via a population of photo-generated holes. This constitutes the first evidence for an ultrafast, nonthermal manipulation of the magnetic order in ferromagnetic semiconductors, thereby opening up fascinating opportunities for future high-speed spin-photon-carrier integrated devices, and above GHz magneto-optical recording.

1:03PM V12.00008 Gate-tunability of electron spin precession in an InGaAs quantum well below an interdigitated ferromagnetic grating, GIAN SALIS, LORENZ MEIER, IBM Research, Zurich Research Laboratory, Saeumerstrasse 4, 8803 Rueschlikon, Switzerland, CHRISTOPH ELLENBERGER, EMILIO GINI, KLAUS ENSSLIN, Solid State Physics Laboratory, ETH Zuerich, 8093 Zuerich, Switzerland — Time-resolved Faraday rotation is used to measure the coherent electron spin precession in a GaAs/InGaAs quantum well below an interdigitated ferromagnetic Fe grating. We show that the electron spin precession frequency can be modified by applying a gate voltage of opposite polarity to neighboring bars. A tunability of the precession frequency of 0.5 GHz/V is observed. Modulating the gate potential at a 1 GHz frequency allows the electron spin precession to be controlled on a nanosecond timescale. Besides the contribution from a spatial displacement of electrons in the inhomogeneous stray field, we also observe spin precession induced by spin-orbit coupling of the moving electrons.

1:15PM V12.00009 Dynamically Decoupled Precession of Interfacial Electron Spins in Fe/AlGaAs (001), GUNTER LUEPKE, HAIBIN ZHAO, DIYAR TALBAYEV, College of William and Mary, AUBREY HANBICKI, CONNIE LI, BERRY JONKER, Naval Research Laboratory — We report on the coherent spin precession dynamics of the interface magnetization in Fe/AlGaAs (001) heterostructures using the time-resolved magnetization-induced second-harmonic generation technique, and compare these results with the bulk spin precession dynamics obtained by time-resolved magneto-optical Kerr effect. We have measured the frequency, phase and hysteretic behavior of the precession dynamics of the interface and bulk. Our results clearly show: (a) the coherent precession of the interface magnetization is decoupled from the bulk magnetization precession even at the picosecond time scale; (b) higher frequency spin precession occurs at the interface than in the bulk; (c) the phase of the interface spin precession is opposite to that of the bulk precession at low fields; and (d) the interface and bulk precession exhibit different hysteretic behavior. This is attributed to different magnetization switching processes and vanishingly small exchange coupling between the interface magnetization and the bulk Fe. The higher precession frequencies observed at the interface for a given field indicate that higher speed performance can be realized in nanoscale magnetic devices where interface properties dominate.

1:27PM V12.00010 Development of an 8-12 GHz variable frequency microwave resonant cavity for optically-detected magnetic resonance (ODMR) of GaAs-related semiconductors, J.S. COLTON, J.R. WIENKES, L.R. OESTREICHER, P.M. SCHRÖDER, University of Wisconsin-La Crosse — In order to do spin echo measurements of the T2 spin coherence time in GaAs and related materials, one must have a resonant microwave cavity; the resonance serves mainly to increase the strength of the magnetic field at the sample. In order to probe materials with g-factors as low as |g| = 0.1 (such as quantum-confined GaAs samples, and bulk/quantum-confined AlGaAs alloys) in moderate magnetic fields (< 7 T), we have selected a resonant frequency of around 10 GHz for the resonator design. In order to fit a 10 GHz cavity into moderately-sized (< 1 inch) magnet bores, however, a high dielectric material must be used, a so-called “dielectric resonator”. We will present the design and testing of such a resonant cavity (resonant mode: TE011), that additionally allows for optical access of the sample, as well as a highly-variable resonant frequency.

1:39PM V12.00011 Simple Model for the Photon Energy Dependence of Optical Nuclear Polarization in GaAs, PATRICK COLES, JEFFREY REIMER, University of California, Berkeley — It was discovered forty years ago that nuclear Zeeman order can be induced by prolonged irradiation of a bulk semiconductor with near-band-gap light. The microscopic mechanism of this optical nuclear polarization process is still under debate. Yet, we are able to predict a major feature of the data, the dramatic photon-energy dependence, from a simple model, irrespective of the spin microscopics. We discuss this model in the context of semi-insulating GaAs.

1:51PM V12.00012 Localization of excitons in Cd$_{1-x}$Mn$_x$Te semimagnetic semiconductors near temperature of phase transition : paramagnetic-spin glass, YURIU GNATENKO, PETRO BUKIVSKIJ, Institute of Physics of NASU — Excitons in semimagnetic semiconductors become trapped by fluctuations of the crystal field as in ordinary solid solution based on II-VI semiconductors. In addition, magnetic-polaron effects are seen in these crystals. These effects stem from an exchange interaction of electrons and holes bound in excitons with d electrons of the magnetic ions. As a result, there is an additional trapping of excitons. At magnetic ion concentration Xc > 0.10 the trapping of excitons not only by fluctuation of the crystal-field potential but also by fluctuations of the crystal magnetization become important. In this paper we are reporting the study of the emission of excitons trapped by magnetization fluctuations at temperatures from 1.8 K to 100 K. Analysis the form and the spectroscopy reveals sub-picosecond demagnetization, precessional trajectory of the magnetization vector, and establishment of the ferromagnetic order on a 100-ps time scale. The dynamic enhancement of the magnetic ordering, manifesting as the photo-induced magnetization below and above the Curie temperature $T_c$, is well explained by a transient increase of $T_c$ via a population of photo-generated holes. This constitutes the first evidence for an ultrafast, nonthermal manipulation of the magnetic order in ferromagnetic semiconductors, thereby opening up fascinating opportunities for future high-speed spin-photon-carrier integrated devices, and above GHz magneto-optical recording.

2:03PM V12.00013 Magnetoplasmon excitations in a quasi-two-dimensional Rashba spintronic systems: Oscillations, resonances, and energy gaps, MANVIR S. KUSHWAHA, Institute of Physics, University of Puebla, Mexico — We report on the theoretical investigation of plasmon excitations in a quasi-two-dimensional electron gas (2DEG) in the presence of a perpendicular magnetic field and spin-orbit (SO) interaction induced by the Rashba effect. We derive and discuss the dispersion relations for charge-density excitations within the framework of Bohm-Pines’ random-phase approximation (RPA). The magnetoplasmons in a 2DEG are known to be characterized by two important properties: (i) the oscillatory behavior of the dispersion curves in the short wavelength limit (SWL), and (ii) the resonance splitting at the frequency $\omega = \omega_{SO}$ in the long wavelength limit (LWL). $n$ being an integer and $\omega_{c}$ the cyclotron frequency. Here we study the effect of the Rashba spin-orbit interactions (SOI) on these characteristics. In our calculations we observe that the SOI modifies drastically both the oscillatory behavior in the SWL and yields multiple resonance splittings, and the Rashba parameter characterizing the SOI.
11:15AM V13.00001 Field-induced spin-solid phases in the spin liquids Tb$_2$Ti$_2$O$_7$ and Nd$_2$Ga$_3$SiO$_{14}$ — CHRISTOPHER WIEBE, National High Magnetic Field Lab, Florida State University, YOUNJUNG JO, HAIDONG ZHOU, EUN SANG CHOI, CHRISTOPHER WIEBE, National High Magnetic Field Laboratory, Florida State University, Tallahassee-FL 32306, USA — Here we report thermodynamic and magnetization measurements at zero and high fields in the pyrochlore Tb$_2$Ti$_2$O$_7$ and in the Kagome lattice Nd$_2$Ga$_3$SiO$_{14}$. In both compounds, previous neutron scattering studies did not reveal any form of magnetic ordering down to the lowest temperatures and have proposed these materials to display a spin-solid ground state [1]. Here we show that heat capacity normalized by temperature down to ~ 350 mK confirms the absence of ordering. Furthermore, magnetization as a function of field at the lowest temperature reveal the existence of an intermediate phase prostruded between the zero field spin-solid and the high-field spin-polarized state. In the case Nd$_2$Ga$_3$SiO$_{14}$ it leads to a 1/2 magnetization plateau for fields along the inter-planar direction, similar to the one recently reported in the pyrochlore compound CdCr$_2$O$_4$ [2]. But for fields along the planes it displays a 1/3 plateau followed by a metamagnetic transition towards a value closer to 4/5. [1] J. S. Gardner et al. Phys. Rev. Lett. 82, 1012 (1999); J. Robert et al., ibid 96, 197205 (2006) [2] H. Ueda, Phys. Rev. Lett. 94, 047202 (2005).

11:27AM V13.00002 Freezing the 2D distorted kagome spin liquid Nd$_2$Ga$_3$SiO$_{14}$ — CHRISTOPHER WIEBE, HAIQONG ZHOU, BRANDON VOGT, JOHN JANIK, Y.-J. JO, LUIS BALICAS, JASON GARDNER, FSU/NHMFL — The distorted kagome system Nd$_2$Ga$_3$SiO$_{14}$ has been investigated with neutron scattering down to 0.04K with no evidence of magnetic long-ranged order of the Nd$^{3+}$ moments in zero field. Substantial diffuse scattering is observed which is consistent with previous measurements of nearest neighbor correlations between the fluctuating spins. Upon the application of a magnetic field in the c-direction, the diffuse scattering is reduced in intensity while magnetic Bragg peaks grow in intensity to saturate by 1 T. The net moment along the c-axis is 1.5(1) $\mu_B$, only 1/3 of the value of the full moment of 3.2 $\mu_B$ per Nd spin, consistent with a 1/2 magnetization plateau in the DC susceptibility. A phase diagram is constructed to denote the boundary between a 2D spin liquid and spin solid phase.

11:39AM V13.00003 Geometric Frustration and Chemical Tuning of Magnetic Order in the Kagome Lattice System YBa$_2$Co$_{11}$O$_{14}$ — JOHN MITCHELL, HONG ZHENG, Materials Science Division, Argonne National Laboratory, LAURENT CHAPON, PAOLO RADAELLI, ISIS, Rutherford Laboratory, ASHIFIA HUQ, Spallation Neutron Source, OAK RIDGE NATIONAL LABORATORY, PETER STEPHENS, SUNY Stonybrook — Transition metal oxides containing a Kagome lattice motif of magnetic ions form the basis for exploring geometric frustration and exotic magnetic ground states. Examples of such systems include pyrochlores, spinels, SrCr$_2$O$_4$, and exotic magnetic ground states. By 1 T. The net moment along the c-axis is 1.5(1) $\mu_B$, only 1/3 of the value of the full moment of 3.2 $\mu_B$ per Nd spin, consistent with a 1/2 magnetization plateau in the DC susceptibility. A phase diagram is constructed to denote the boundary between a 2D spin liquid and spin solid phase.

11:51AM V13.00004 Magnetic Phase Diagram of Co$_3$V$_2$O$_8$ — FEI YEN, BERND LORENZ, Y. Q. WANG, Y. Y. SUN, C. W. CHU, University of Houston/TCSUH — Kagomé-staircase lattice structures like Ni$_3$V$_2$O$_8$ and Co$_3$V$_2$O$_8$ have recently attracted attention because of their complex magnetic phase diagrams and the magnetically induced ferroelectric (FE) phase observed in Ni$_3$V$_2$O$_8$. Co$_3$V$_2$O$_8$ at zero magnetic field exhibits five subsequent magnetic phase transition in a narrow temperature range. It has an incommensurate antiferromagnetic phase below $T_n$=11.4 K and weak ferromagnetic behavior along the a-axis at $T_c$=6.2 K. Along with three other phase transitions in between, $T_1$=8.9 K, $T_3$=7.0 K and $T_4$=6.9 K, the evolution of these five phase transitions under magnetic field, phase boundaries, is traced through magnetic susceptibility and dielectric constant anomalies. We resolve the complete magnetic phase diagram of Co$_3$V$_2$O$_8$ with the magnetic field applied along the principal crystallographic orientations.

12:03PM V13.00005 Field dependence of the magnetic order in Co$_3$V$_2$O$_8$ — YING CHEN, NIST Center for Neutron Research and University of Maryland, J. W. LYNN, Q. HUANG, F. M. WOODWARD, T. YILDIRIM, NIST Center for Neutron Research, G. LAWES, Wayne State Univ., A. P. RAMIREZ, Bell Labs, N. ROGADO, Princeton Univ. and DuPont Central Research and Development, R. J. CAVA, Princeton Univ., A. AHRARONY, O. ENTIN-WOHLMAN, Tel Aviv Univ. and Ben Gurion Univ., A. B. HARRIS, University of Pennsylvania — Co$_3$V$_2$O$_8$ (CVO) has a geometrically frustrated magnetic lattice, a Kagomé' staircase. In zero field [1], CVO initially orders magnetically at 11.3 K into an incommensurate phase, with wave vector $k=(\delta,0,\delta)$ with $\delta=0.55$. $\delta$ decreases monotonically with decreasing temperature. It locks into a commensurate antiferromagnetic phase of $1/2$ and $1/4$ below the ferromagnetic ground state ($\delta=0$) is revealed at 6.2 K. The spin direction for all spins is along the a axis. A theory based on a minimal Ising model with competing exchange interactions can explain the basic features of the magnetic ordering. The application of magnetic field along the a axis strongly affects all of the phases. In particular, the ferromagnetic state is suppressed in favor of the $\delta=0.5$ antiferromagnetic state. [1] Y. Chen, J. W. Lynn, Q. Huang, F. M. Woodward, T. Yildirim, G. Lawes, A. P. Ramirez, N. Rogado, R. J. Cava, A. Aharony, O. Entin-Wohlman, and A. B. Harris, Phys. Rev. B 74, 014430 (2006).

12:15PM V13.00006 High-Energy Magneto-Dielectric Effect in Co$_3$V$_2$O$_8$ — L. I. VERGARA, R. C. RAI, J. CAO, S. BROWN, J. L. MUSFELDT, University of Tennessee, D. J. SINGH, Oak Ridge National Laboratory, G. LAWES, Wayne State University, N. R. GADGET, DuPont Central Research and Development, R. J. CAVA, Princeton University, X. WEI, Florida State University — We investigate the optical and magneto-optical properties of the Kagomé staircase compound Co$_3$V$_2$O$_8$ in order to explore mechanistic aspects of the high-energy magneto-dielectric effect. Co$_3$V$_2$O$_8$ displays a much smaller dielectric contrast compared to quasi-isosctructural Ni$_3$V$_2$O$_8$, a result that we attribute to a high-temperature local structural distortion in Co$_3$V$_2$O$_8$ along the cross-tie direction. Such a distortion prevents the low temperature magnetic transitions from having a strongly coupled layer component. This proposition is supported by vibrational studies.

1 This work is supported by the U.S. Department of Energy.
12:27PM V13.00007 A Microscopic Model of Magnetoelectric Interactions in Ni3V2O8, TANER YILDIRIM, NIST Center for Neutron Research, A. B. HARRIS, University of Pennsylvania, A. AHARONY, O. ENTIN-WOHLMAN, Tel Aviv University, Israel — We develop a microscopic magnetoelectric coupling in Ni3V2O8 (NVO) which gives rise to the trilinear phenomenological coupling used previously to explain the phase transition in which magnetic and ferroelectric order parameters appear simultaneously. Using combined neutron scattering measurements and first-principles calculations of the phonons in NVO, we determine eleven phonons which can induce the observed spontaneous polarization. Among these eleven phonons, we find that a few of them can actually induce a significant dipole moment. Using the calculated atomic charges, we find that the required distortion to induce the observed dipole moment is very small (~0.001 Å) and therefore it would be very difficult to observe the distortion by neutron-powder diffraction. Finally, we identify the derivatives of the exchange tensor with respect to atomic displacements which are needed for a microscopic model of a spin-phonon coupling in NVO and which we hope to obtain from a fundamental quantum calculation such as LDA+U.

12:39PM V13.00008 Synthesis and characterization of thin film Ni$_3$V$_2$O$_8$, G. LAWES, C. SUDAKAR, P. KHAREL, R. NAIK, Wayne State University — We have prepared thin films of multiferroic Ni$_3$V$_2$O$_8$ using sputter deposition and spin coating techniques. Raman spectroscopy and XRD confirm that the as-deposited films are amorphous, single-phase Ni$_3$V$_2$O$_8$. These films develop increasing crystalline order on annealing at 900 °C, although they remain polycrystalline. These thin film Ni$_3$V$_2$O$_8$ samples develop a net magnetization below T=4 K; this temperature is consistent with the magnetic transition in bulk samples. We observe an anomaly in the dielectric constant coincident with this magnetic transition. Despite being able to apply an electric field of over 6 MV/m to these samples, we are unable to observe any voltage-induced shift in this anomaly. We will discuss the implications of these results for future studies on thin film multiferroics.

12:51PM V13.00009 Thermal expansion and pressure effect in the Kagome-staircase compound Ni$_3$V$_2$O$_8$, R. CHAUDHURY, F. YEN, C. R. DELA CRUZ, B. LORENZ, Y. Q. WANG, Y. Y. SUN, C. W. CHU, UCSUH and Dept. of Physics, University of Houston — Ni$_3$V$_2$O$_8$ has attracted attention because of its ferroelectricity (FE) induced by a helical magnetic order. Strong spin-lattice interaction is necessary to explain the ionic displacements leading to FE. To reveal the signature of lattice strain associated with the ferroelectric transitions we have conducted high-resolution thermal expansion measurements along the a, b, c axes. The strongest lattice anomalies are observed at the low-temperature (3.9 K) lock-in transition from the incommensurate helical magnetic modulation into a commensurate magnetic structure. The stability of the FE with respect to lattice strain as induced by hydrostatic pressure was investigated by measuring the dielectric constant and the ferroelectric polarization under pressures up to 2 GPa. The pressure-temperature phase diagram of Ni$_3$V$_2$O$_8$ is determined. The low-temperature commensurate phase in Ni$_3$V$_2$O$_8$ is stabilized under pressure and the ferroelectricity is completely suppressed above a critical pressure of 1.64 GPa.

1 Supported by the T.L.L. Temple Foundation, the J.J. and R. Moores Endowment, the State of Texas through TCSUH, and at LBNL by the DOE.
2 also at: LBNL, Berkeley and HKUST, Hong Kong

1:03PM V13.00010 Optical Properties and Magnetic Field-Induced Phase Transitions in the Ferroelectric State of Ni$_3$V$_2$O$_8$, R. C. RAI, J. CAO, S. BROWN, J. L. MUSFELDT, University of Texas, A. KASHINATHAN, UC Davis, D. J. SINGH, ORNL, G. LAWES, Wayne State University, N. ROGADO, DuPont, R. J. CAVA, Princeton University, X. WEI, NHMFL — We present a combination of optical spectra, first principles calculations, and magneto-optical measurements to elucidate the electronic structure and to study the phase diagram of Ni$_3$V$_2$O$_8$. We find a remarkable interplay of magnetic field and optical properties that reveals additional high magnetic field phases and an unexpected electronic structure which we associate with the strong magnetoelectric di-couplings in this material over a wide energy range. Specifically, we observed several prominent magneto-dielectric effects that derive from changes in crystal field environment around Ni spine and cross-tie centers. This effect is consistent with a field-induced modification of local structure. We find Ni$_3$V$_2$O$_8$ to be an intermediate gap, local moment band insulator. This electronic structure is particularly favorable for magneto-electro-couplings, because the material is not subject to the spin charge separation characteristic of strongly correlated large gap Mott insulators, while at the same time remaining a magnetic insulator independent of the particular spin order and temperature.

1:15PM V13.00011 Magnetodielectric coupling in Mn$_2$O$_4$ and MnCr$_2$O$_4$, T. RACKETT, Wayne State University, E. TOBERER, R. SESHADRIN, UC Santa Barbara, G. LAWES, Wayne State University — We have investigated the temperature and magnetic field dependent dielectric constants of the ferrimagnetic insulators Mn$_2$O$_4$ and MnCr$_2$O$_4$. We have also measured the heat capacity and AC magnetic susceptibility through the multiple spin ordering transitions in these materials. At the zero field T = 42 K and T = 35 K magnetic transitions in Mn$_2$O$_4$ we observed sharp drops in the dielectric constant. In an applied field of 5 kOe, Mn$_2$O$_4$ shows a positive shift in dielectric constant at the intermediate T = 40 K transition in addition to the features observed at zero field. MnCr$_2$O$_4$ also shows features in the dielectric constant at the magnetic transitions at T = 40 K and T = 28 K, though these shifts were approximately 100 times smaller than those observed in Mn$_2$O$_4$. These results will be discussed in the framework of models for coupling the dielectric constant to non-colinear long-range magnetic order.

1:27PM V13.00012 Ab-initio studies of electronic properties of chalcogenide spinels, M. MAIRBEK CHSHIEV, Y.-H. A. WANG, ARUNAVA GUPTA, Center for Materials for Information Technology, University of Alabama, Tuscaloosa, AL, JOANNA BETTINGER, YURI SUZUKI, Department of Materials Science and Engineering, UC Berkeley, Berkeley, CA, WILLIAM H. BUTLER, Center for Materials for Information Technology, University of Alabama, Tuscaloosa, AL — Cu$_2$Cr$_2$Se$_4$ is a normal chalcogenide spinel which exhibits ferromagnetic properties including a relatively high Curie temperature of 450 K [1] which makes it a promising candidate for use in spintronics devices. Another chalcogenide spinel of enhanced interest for spintronics is CdCr$_2$Se$_4$, which seems to be a promising ferromagnetic semiconductor for electrical spin injection into III-V device heterostructures [2]. We report first principles calculations of the electronic structure of substoichiometric Cu$_2$Cr$_2$Se$_{3.7}$ and Cu$_2$Cd$_{1.9}$Cr$_{0.1}$Se$_4$ spinels. The calculations were performed using the Vienna ab-initio simulation program (VASP) with the Generalized Gradient Approximation (GGA) of Density Functional Theory (DFT). Our calculations indicate that both Se deficient Cu$_2$Cr$_2$Se$_{3.7}$, as well as Cu$_2$Cd$_{1.9}$Cr$_{0.1}$Se$_4$ show half-metallic behavior over a wide range of $x$ with a gap around the Fermi level in the minority density of states. [1] P.K. Lotgering, Solid State Commun. 2 (1964) 55 [2] G. Kioseoglou et al., Nature Materials 3 (2004) 799

1:39PM V13.00013 Magnetic anisotropy and geometrical frustration in the Ising spin-chain system Sr$_5$Rh$_4$O$_{12}$, G. LAWES, S. BROWN, J. L. MUSFELDT, University of Texas, A. B. HARRIS, University of Pennsylvania, A. AHARONY, O. ENTIN-WOHLMAN, Tel Aviv University, Israel — The magnetic anisotropy and geometrical frustration in the Ising spin-chain system Sr$_5$Rh$_4$O$_{12}$ consists of a triangular lattice of spin chains running along the c-axis. It is antiferromagnetically ordered below 23 K with the intrachain and interchain coupling being ferromagnetic (FM) and antiferromagnetic (AFM), respectively. There is strong evidence for an Ising character in the interaction and geometrical frustration that causes incomplete long-range AFM order. The isofield magnetization exhibits two-step-like transitions leading to a ferrimagnetic state at 2.4 T and a FM state at 4.8 T, respectively. Sr$_5$Rh$_4$O$_{12}$ is a unique frustrated spin-chain system ever found in 4d and 5d based materials without a presence of an incomplete 3d-electron shell.

1 This work was supported by NSF grants DMR-0240813, DMR-0552267 and DOE grant DE-FG02-98ER45707.
1:51PM V13.00014 Antiferromagnetism and geometrical frustration in one-dimensional Ca₃Ir₂O₁₂ and Ca₃IrO₆ single crystals\footnote{This work was supported by NSF grants DMR-0240813, DMR-0552267 and DOE grant DE-FG02-98ER45707.}, ANGELA DOUGLASS, VINOBALAN DURAIJ, SHALINEE CHIKARA, GANG CAO, Department of Physics and Astronomy, University of Kentucky, Lexington, KY40506, SEAN PARKIN, Department of Chemistry, University of Kentucky, Lexington, KY40506, PEDRO SCHLOTTMANN, Department of Physics, Florida State University, Tallahassee, FL32306 — We report a structural, thermodynamic and transport study of the newly synthesized single crystal Ca₃Ir₂O₁₂ and Ca₃IrO₆. Both materials consist of a triangular lattice of spin chains running along the c-axis. Ca₃Ir₂O₁₂ and Ca₃IrO₆ are antiferromagnetically ordered below 7.8 K and 12 K, respectively. The study reveals an unusually large ratio of the Curie-Weiss temperature to the Neel temperature (> 36 for Ca₃Ir₂O₁₂) and a small entropy removal associated with the magnetic phase transition. In addition, the magnetic susceptibility and heat capacity show that the phase transition is essentially insensitive to the application of the magnetic field. All results suggest the presence of the geometrical frustration that causes incomplete long-range antiferromagnetic order. The results will be presented and discussed along with comparisons drawn with other related systems.

2:03PM V13.00015 Configurational Electronic Entropy and the Phase Diagram of Mixed-Valence Oxides: The Case of LiₓFePO₄ \footnote{X. Wu, O. Diéguez, K. Rabe and D. Vanderbilt, Phys. Rev. Lett. 97, 107602 (2006).}, FEI ZHOU, THOMAS MAXISCH, GERBRAND CEDER, Department of Materials Science and Engineering, MIT — We demonstrate that configurational electronic entropy, previously neglected, in \textit{ab initio} thermodynamics of materials can qualitatively modify the finite-temperature phase stability of mixed-valence oxides. While transformations from low-T ordered or immiscible states are almost always driven by electronic, rather than ionic configurational entropy. We argue that such an electronic entropic mechanism, rather than an ionic one, may be relevant to most other mixed-valence systems. Details in Phys. Rev. Lett. 97, 155704 (2006)

Thursday, March 8, 2007 11:15AM - 1:51PM —
Session V20 DMP: Focus Session: Superlattices and Oxides on Silicon

11:15AM V20.00001 Tailoring the properties of artificially layered ferroelectric superlattices \footnote{X. Wu, O. Diéguez, K. Rabe and D. Vanderbilt, Phys. Rev. Lett. 97, 107602 (2006).}, MATTHEW DAWBER, NICOLAS STUCKI, CELINE LICHTENSTEIGER, STEFANO GARIGLIO, JEAN-MARC TRISCONE, DPMC, University of Geneva, Switzerland — A key attraction of artificial ferroelectric superlattices is the potential to be able to tailor the properties of the material to a particular application. Here we demonstrate that the key ferroelectric parameters, polarization and critical temperature can be tuned over a very large range in PbTiO₃/SrTiO₃ superlattices by varying the ratio of the layer thicknesses. It is shown that the polarization can be tuned from 0-60 \(\mu\)C/cm\(^2\) and the transition temperature from room temperature to 700\(^\circ\)C while maintaining a perfect crystal structure and low leakage currents in these heterostructures. We developed a simple model based on Landau theory that would guide straightforward production of samples with ferroelectric properties designed for particular applications. We also explore the phase transition behaviour with temperature in superlattices with very thin PbTiO₃ layers where we find not only unexpected evidence of ferroelectricity but also an unusual relationship between strain and polarization.

11:27AM V20.00002 Electrostatics of superlattices by first principles \footnote{D. D. Fong et al. PRB 71, 144112 (2005).}, XIFAN WU, Princeton University, OSWALDO DIÉGUEZ, Massachusetts Institute of Technology, MASSIMILIANO STENGEL, U.C. Santa Barbara, KARIN RABE, DAVID VANDERBILT, Rutgers University — A complete theory of epitaxial perovskite superlattices requires an understanding of both epitaxial strain effects and of electrostatic boundary conditions. Here, focusing on the latter issue, we have carried out first-principles calculations of the nonlinear dielectric properties of short-period BaTiO₃/SrTiO₃ and PbTiO₃/SrTiO₃ superlattices having the in-plane lattice constant of SrTiO₃. In particular, we have calculated the layer polarizations \(p_j\) as defined using the Wannier-based method of Wu, Diéguez, Rabe and Vanderbilt\cite{wu2006} for each neutral BaO, SrO, PbO, or TiO\(_2\) layer, and modeled \(p_j\) as a function of displacement field \(D\) (which is uniform throughout the superlattice), the chemical identity of the layer itself, and the chemical identity of its near neighbors. We then test our expectation that the dependence on the identity of neighboring layers should decay rapidly with distance. If we apply a cut-off to the range of this interlayer interaction, we arrive at a model description that allows us to predict \(p_j(D)\) for each layer, and thus the overall \(P(D)\) (and trivially, also \(P\) vs. electric field and related quantities) for a superlattice of arbitrary layer sequence.

11:39AM V20.00003 Interfacial Intermixing in Ferroelectric Superlattices from First Principles \footnote{D. D. Fong et al. PRB 71, 144112 (2005).}, VALENTINO R. COOPER, Rutgers University, KAREN JOHNSTON, Helsinki University of Technology, KARIN M. RABE, Rutgers University — Ferroelectric superlattices present a unique foundation for creating novel materials for modern devices. In ideal superlattices with perfectly flat, compositionally abrupt interfaces, first-principles studies have shown how factors such as strain due to lattice mismatches, charge compensation and bonding at the interface can be controlled to enhance the ferroelectric properties of the superlattice. In real superlattices, the presence of an additional factor, cation intermixing at the interface, is suggested by high-resolution COBRA studies\cite{fong2007}. As the period of a superlattice decreases, the effect of this intermixing would be expected to become increasingly important. Here, we present results of a first-principles study of the effect of interfacial intermixing on short-period \(x_{FT}/y_{ST}\) superlattices. We find that the effect of intermixing on the superlattice polarization can indeed be substantial, and use first-principles information about atomic and electronic properties to interpret and model the effect. Implications for other superlattice combinations and experiments will be discussed.
Interfaces play a pivotal role in the properties of complex oxides such as polarization of ferroelectrics, band offsets of gate dielectrics and the field effect in correlated electron materials. The concept of the interface phase has guided us in understanding these diverse roles of the interface. Moreover, this concept is especially powerful in guiding the development of processes for the heteroepitaxial growth of oxides on semiconductors. Functional substitutions of the most polar perovskite-oxide SLs that can be grown on currently available substrates. This flexible modeling procedure can be applied to a wide variety of layered perovskite-oxide nanostructures, providing guidance for experimental development of nanoelectromechanical devices with substantially improved polar properties.

Work done in collaboration with K. Rabe and D. Vanderbilt, and supported by the Center for Piezoelectrics by Design (CPD) under ONR Grant N00014-01-1-0365.

1:15PM V20.00007 Surface morphology of PbTiO$_3$ films on SrTiO$_3$ (001) . K. LATIFI, CAROL THOMPSON, Physics Dept., Northern Illinois University, D. D. FONG, B. B. STEPHENSON, P. H. FUOSS, J. A. EASTMAN, F. JIANG, Materials Science Division, Argonne National Laboratory, S. K. STREIFFER, R.-V. WANG, Center for Nanoscale Materials, Argonne National Laboratory — Strain relaxation is a ubiquitous process in the synthesis of heteroepitaxial films. Films deposited onto a substrate with a small lattice parameter mismatch will often initially form as coherently strained (lattice matched) layers. As the film grows and exceeds a critical thickness, the stored elastic energy is released through the creation of crystal defects such as misfit dislocations. Even before dislocation introduction, epitaxial strain can lead to morphological instabilities of the growth interface, with the formation of mounds. We use atomic force microscopy to investigate surface morphology related to strain relaxation during the epitaxial growth of PbTiO$_3$ films ranging from 10 nm to 385 nm in thickness on SrTiO$_3$ (001) substrates. The ferroelectric phase transition temperature of coherently strained PbTiO$_3$ films is increased, but also depends on thickness. Therefore, for some range of typical growth temperatures of organo-metallic vapor phase epitaxy, it is possible for the film to undergo a paraelectric to ferroelectric phase transition during growth. This could lead to additional mechanisms of strain relaxation becoming active during growth.

The authors acknowledge the funding support from the grant through the Army Research Laboratory (Award No. DAAD19-03-2-0017).

12:51PM V20.00008 Ferroelectricity in ultra-thin and thick ferroelectric films of Pb$_{1-x}$Sr$_{0.65}$TiO$_3$ studied by second harmonic generation . SHIWEI LIU, JACQUES CHAKHALIAN, MIN XIAO, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, CHONGLIN CHEN, Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, Texas 78249 — Second harmonic generation (SHG) measurements were performed in the reflection geometry using the femtosecond Ti:Sapphire pulse laser at the wavelength of 810 nm for a 16-nm-thick ultra-thin Pb$_{0.35}$Sr$_{0.65}$TiO$_3$ film and a 243-nm-thick Pb$_{0.35}$Sr$_{0.65}$TiO$_3$ film, which were epitaxially deposited on (001) MgO substrates by pulsed laser ablation (PLD). It is concluded that in the ultra-thin film the ferroelectric phase is still present and a remarkably sharp ferroelectric phase transition was observed. In contrast, the thick film exhibits a pronounced diffuse phase transition. Theoretical analysis based on the polarization diagrams show the compensated c-domain fraction is dominant in both films whereas the nonlinear susceptibility of the ultra-thin film has a different tensor property from the thick film.

12:39PM V20.00006 Ferroelectricity and Polarization-Dependent Tunneling in BaTiO$_3$ Films Below 10 Layers . ARTHUR P. BADDORF, JUNSOO SHIN, SERGEI V. KALININ, Oak Ridge National Laboratory, VON BRAUN NASCIMENTO, E. WARD PLUMMER, University of Tennessee — Predictions for the minimum critical film thickness for ferroelectricity have continuously decreased. For BaTiO$_3$, ferroelectricity has previously been observed experimentally down to 12 layers and predicted by first-principles calculations in 6 layer films. We have examined BaTiO$_3$ ultra-thin films grown on SrRuO$_3$/SrTiO$_3$ using laser-MBE in high oxygen pressures and report evidence of a ferroelectric state at room temperature by in-situ characterization of structure, using low energy electron diffraction (LEED I-V) and by scanning tunneling spectroscopy (STS). Films produce sharp (1x1) LEED patterns, indicating well-ordered tetragonal phase structure. Comparison of observed diffraction intensities for 4 and 10 layer films at 130 and 300 K with calculated intensities reveals a vertical displacement of the central Ti, consistent with a polarization associated with compressive strain. Reversible polarization switching was observed locally as a jump in the electron tunneling current at +/- 2.5 V using a scanning tunneling microscope. Research was sponsored by the Division of Materials Sciences and Engineering and the Center for Nanophase Materials Sciences, Office of Basic Energy Sciences, U.S. Department of Energy with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC.

11:51AM V20.00004 Understanding, enhancing and fine-tuning polar properties in multicomponent perovskite superlattices . SERGE NAKHMANSON, Argonne National Laboratory — Modern epitaxial thin-film techniques make it possible to synthesize artificial multicomponent perovskite-oxide superlattices (SLs) with interfaces that are atomically flat and compositionally abrupt. The behavior of such systems is dominated by strong interactions between individual SL layers, high levels of epitaxial strain and symmetry lowering relative to the bulk. All of these factors can be manipulated in order to enhance or custom-tailor the useful polar properties — such as polarization and piezoelectric response — for a wide variety of technological applications. First-principles computational techniques are a tool of choice to help us understand how the strain, symmetry and composition of these complex systems influence their polar properties. However, the prohibitive computational costs associated with such simulations, growing rapidly with the period of the SL increases, make it impossible to answer some broader, more interesting questions: in particular, how could the SL layer arrangement be optimized to obtain the best possible polar properties? Here we show how first-principles calculations combined with a simple model for SL polarization and a genetic-algorithm optimization allow us to find answers to the questions mentioned above and, among other things, to predictively identify the most polar perovskite-oxide SLs that can be grown on currently available substrates. This flexible modeling procedure can be applied to a wide variety of layered perovskite-oxide nanostructures, providing guidance for experimental development of nanoelectromechanical devices with substantially improved polar properties.

Work done in collaboration with K. Rabe and D. Vanderbilt, and supported by the Center for Piezoelectrics by Design (CPD) under ONR Grant N00014-01-1-0365.

12:27PM V20.00005 ABSTRACT WITHDRAWN
11:15AM V25.00001 Spin Response in Organic Spin-Valves based on LSMO Electrodes\textsuperscript{1}, FUJIAN WANG, CUNGENG YANG, Department of Physics, University of Utah, Z. VALY VARDENY, Department of Physics, University of Utah, XIAOGUANG LI, Heifei National Laboratory for Physical Sciences at Microscale and Department of Materials Science & Eng, University of Science and Technology of China, VARDENY’S GROUP TEAM, XIAOGUANG LI’ GROUP COLLABORATION — We fabricated spin-valves made of organic semiconductor (OSEC) thin films sandwiched between ferromagnetic La$_2/3$Sr$_{1/3}$MnO$_3$ (LSMO) and cobalt electrodes, using several OSEC small molecules. We measured the temperature (T) and voltage bias (V) dependence of the spin-valve related giant magneto-resistance (GMR) effect. We found a universal GMR decrease with T, where the GMR completely diminishes at $\sim 275^\circ$K regardless of the OSEC layer. We show evidence that the underlying mechanism for the GMR decrease with T is the decrease in the spin injection capability of the LSMO electrode. We also found that the GMR steeply decreases with V, and is asymmetric respect to the applied voltage direction.

\textsuperscript{1}Supported in part by grants from the DOE and the NSF DMR at the University of Utah.

11:27AM V25.00002 Spin Valve Effects in Hybrid Organic-Inorganic Devices\textsuperscript{1}, YAOHUA LIU, TAEG-WEON LEE, HOWARD E. KATZ, DANIEL H. REICH, The Johns Hopkins University — Magnetoelectronic devices based on organic semiconductors (OSC) hold promise due to the long spin coherence in these materials and the ability to tune relevant properties such as carrier mobility and interface barriers via organic synthesis. We have studied spin valve effects in vertical geometry organic/inorganic devices, using Fe and Co as the bottom and top electrodes. Several different organic semiconductors, including Perylenetetracarboxylic dihydride (PTCDA) and the previously studied Alq3, have been used as the spin transport layers. At low temperatures, up to 5\% positive hysteretic magnetoresistance (MR) has been observed at low field in devices with semiconductor thickness of 140 nm, which is much larger than the tunneling limit. The MR decreases as the bias voltage or current increases. Possible mechanisms for spin-polarized transport in these devices and prospects for synthesis of materials with improved performance will be discussed.

\textsuperscript{1}Work Supported by NSF Grant No. DMR-0520491.

11:39AM V25.00003 Morphology Influenced Properties in Organic Semiconducting Thin Films for Spin-Valves\textsuperscript{1}, J. SHEUNG, M. TEAGUE, C.R. HUGHES, S. MITROVIC, N.-C. YEH, Department of Physics, California Institute of Technology, Pasadena CA 91125 — The physical and electronic properties influenced by the morphology in organic thin films of tris(8-hydroxyquinoline) aluminum (Alq3) have been investigated systematically. This material is of interest for spintronics as the tunneling barrier in spin valves and as optoelectronics because it exhibits electroluminescence. In particular, in vacuo vapor deposited thin films are studied by atomic force microscopy, scanning tunneling microscopy and tunneling spectroscopy to determine the spatially resolved correlation of the electronic properties with the morphology. The contributions of various coulombic and thermodynamic parameters to achieving smooth and monolayer thick Alq3 films are also investigated. Additionally, various high Curie temperature ferromagnets, including La$_{1.8}$Sr$_{1/5}$MnO$_3$, are explored as the spin-polarized electrode for optimized spin and charge transport properties in the organic/ferromagnetic heterostructures.

\textsuperscript{1}This work is supported by NSF under the Center for Science and Engineering of Materials at Caltech.

11:51AM V25.00004 Dipolar-Biased Tuning of Magnetization in Crystals of Single Molecule Magnets, KUNIO AWAGA, Nagoya Univ. — The molecular cluster Mn12 has attracted much interest as a single-molecule magnet (SMM) and as a multi-redox system. It has a high-spin ground state of $S=10$ and a strong uniaxial magnetic anisotropy, and the combination of the two natures makes an effective potential barrier between the up and down spin states. At low temperatures, the magnetization curve exhibited a hysteresis loop and the quantum tunneling of magnetization (QTM). In the present study, we investigated the magnetic properties of the mixed-metal SMM, Mn11Cr, through the analysis of Mn11Cr/Mn12 mixed crystal. High-frequency EPR spectra were well explained by assuming that Mn11Cr was in a ground spin-state of $S=19/2$ with nearby the same EPR parameter set as for Mn12. QTM in Mn11Cr was observed with the same field interval as for Mn12. The magnetization of Mn11Cr and Mn12 in the mixed crystal can be independently manipulated by utilizing the difference between their coercive fields. The resonance fields of QTM in Mn11Cr are significantly affected by the magnetization direction of Mn12, suggesting the effect of dipolar-biased tunneling. Besides SMM, we would also like to report the unusual magnetic properties of spherical hollow nanomagnets, the electrical properties of heterochiral thiazyli radicals, and their possible applications in spintronics and organic electronics.

12:27PM V25.00005 Regioregular polythiophene based spintronic devices: effect of interface\textsuperscript{1}, RONALD OSTERBACKA, Abo Akademi University, SAYANI MAJUMDAR, Abo Akademi University and University of Turku, HIMALDRAJ MADUMDAR, Abo Akademi University, REINO LAIHO, PEKKA LAUKKANEN, University of Turku, JUHANI VAYRYNEN, juhanv.vayrynen@utu.fi — Polymeric spin valves have been fabricated using regio-regular (poly-3-hexylthiophene) (R3P3HT) as the spacer layer sandwiched between La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) and Co electrodes. The devices show high spin valve magnetoresistance (MR) at 5K (80\%) which reduces at room temperature to 1.5\%. The spin valve behavior is quite similar to a magnetic tunnel junction although the non-magnetic spacer layer ($\sim 100$ nm) is much thicker than the tunneling limit. We attribute this behavior to the formation of a thin spin-selective tunneling interface between LSMO and R3P3HT caused by the chemical bonding between R3P3HT and LSMO as observed by x-ray photoelectron spectroscopy measurement. Deliberate destruction of the spin injecting interface by the introduction of a monolayer of organic insulators between LSMO and R3P3HT reduces the spin injection.

\textsuperscript{1}Academy of Finland and Magnus Ehrnrooth foundation is acknowledged for financial support.
12:39PM V25.00006 Ferrimagnetic resonance study on photo-induced magnetism in hybrid magnetic semiconductor V(TCNE)$_2$, $x \sim 2$ film$^1$, JUNG-WOO YOO, R. SHIMA EDELSTEIN, D. M. LINCOLN, A. J. EPSTEIN, The Ohio State University — The V(TCNE)$_2$, $x \sim 2$ is a fully spin-polarized magnetic semiconductor, whose magnetic order exceeds room temperature ($T_c > 350$ K), and electronic transport follows hopping mechanism through the Coulomb energy split $\pi$ subband. In addition, it was determined that this material has thermally reversible persistent change in both magnetism and conductivity driven by the optical excitation $[1]$. Here, we report detailed investigation on photo-induced magnetism in V(TCNE)$_2$, by employing ferrimagnetic resonance (PIFMR) study with an in-situ light illumination. Upon optical excitation ($\lambda > 457.9$ nm), the FMR spectra display substantial change in their linewidth and resonance field. Angular dependence analyses of line shift indicate the increase of uniaxial anisotropy field in the film caused by the light irradiation. The results demonstrated that the change in overall magnetic anisotropy by the illumination plays an important role in inducing photo-induced magnetism in (TCNE)$_2$ class magnet.

$^1$Supported in part by AFOSR Grant No. F49620-03-1-0175 and FA9550-06-1-0175 and DOE Grant No. DE-FG02-01ER45931 and DE-FG02-01ER45271.

12:51PM V25.00007 On the Mechanism Causing Large Room-Temperature Magnetoresistance in OLEDs, Y. SHENG, T. NGUYEN, Dept. of Phys. & Astr., Univ. of Iowa, G. VEERARAGHAVAN, Dept of Elec. & Comp. Engr., Univ. of Iowa, J. RYBICKI, Dept. of Phys. & Astr., Univ. of Iowa, O. MERMER, Univ. of California, Santa Barbara, M. WOHLGENANNT, Dept. of Phys. & Astr., Univ. of Iowa — We report on the experimental study of a recently discovered, large room-temperature magnetoresistance effect in sandwich devices comprised of nonmagnetic electrodes and various organic semiconductor thin films. The effect reaches up to 10% in a magnetic field of 10 mT at room temperature and saturates at fields larger than several tens of milliTeslas. In materials with strong spin-orbit coupling the characteristic magnetic field scale shifts to fields that are 10-100 times larger, consistent with the spin-orbit coupling strength. Our experiments therefore show that the organic magnetoresistive effect is caused by spin-dynamics, possibly induced by the hyperfine interaction. We discuss two recently proposed models to explain the organic magnetoresistive effect, which are based on spin-dependent exciton formation and spin-dependent hopping, respectively.

1:03PM V25.00008 Molecular Beam Epitaxy Growth of Organic Spin Valves$^1$, K. PI, W. RANG, R. THAMANKAR, Y. CHYE, Y. F. CHIANG, Y. LI, R. K. KAWAKAMI, UC Riverside, Department of Physics and Astronomy — Spin-polarized transport across organic semiconductors has recently been demonstrated in organic spin valves consisting of ferromagnet(FM)/Alq$_3$/FM trilayers $[a]$. Organic semiconductors are interesting for spintronics due to their low spin-orbit coupling (which could in principle be tuned via chemical synthesis) and opto-electronic coupling to spin. We are utilizing molecular beam epitaxy (MBE) deposition through shadow masks to fabricate Co/Alq$_3$/Fe devices on MgO(001) substrates. Furthermore, we have developed the capability to perform variable temperature magnetotransport measurements without removing the sample from UHV. We find that for Alq$_3$ thickness below 100 nm, the sample exhibits linear I-V curves indicating a short across the Alq$_3$ layer, consistent with previous studies $[a]$. This is likely due to the interdiffusion of Co as the top electrode is deposited onto the Alq$_3$. By employing cryogenic techniques during top electrode growth, we are able to reduce the effects of Co diffusion and the formation of pinholes. We will report our progress on the in situ magnetotransport measurements to investigate spin-polarized transport in our devices.

$^1$Supported by ONR, NSF, the Research Corporation, and CNID.

1:15PM V25.00009 Boosting quantum efficiency of single layer organic light emitting device by doping CoFe magnetic nanoparticles$^1$, CHENGJUN SUN, Materials Science and Technology Division, Oak Ridge National Laboratory, YUE WU, ZHIHUA XU, BIN HU, Department of Materials Science and Engineering, University of Tennessee, JIAN-PING WANG, The Center for MINT, and Department of ECE, University of Minnesota, JIAN SHEN, Materials Science and Technology Division and Center for Nanophase Materials Science Division, Oak Ridge National Laboratory — The effects of doping magnetic CoFe nanoparticles on electroluminescence (EL) efficiency vs. current density, and current density vs. applied voltage for single layer organic light emitting devices (OLEDs) have been investigated. The electron trap densities increased with the increase of CoFe dopants, resulting in a high trap-filled limit (TFL) threshold voltage and significant enhancement EL efficiency $(\sim 27\%)$. The EL efficiencies were further improved $(\sim 5-7\%)$ by applied magnetic field. These improvements could be attributed to the enhancements of the ratios of the formation of excitons, and singlets to triplets, respectively and simultaneously. A maximum 32% enhancement combing the two effects in EL efficiency has been achieved.

$^1$This research is sponsored by the LDRD Program of ORNL, managed by UT-Battelle, LLC for the U. S. Department of Energy under Contract No. DE-AC05-00OR22725.

1:27PM V25.00010 Spin dynamics of photoexcited polarons in MEH-PPV: optically detected magnetic resonance studies$^1$, CUNGENG YANG, ZEEV VARDENY, University of Utah, EITAN EHRENFREUND, Technion University — We studied the full dynamics of the photoluminescence detected magnetic resonance (PLDMR), photoinduced absorption (PA), and PA detected magnetic resonance (PADMR) in MEH-PPV films, as a function of microwave power, $P$, and modulation frequency, $f_m$. We found it critically important to measure both in-phase and quadrature components; otherwise key characteristics of the dynamics are not unraveled. For example, the PLDMR in-phase component changes sign at $f_m < f_0$ of about 30 kHz before decaying at higher frequencies. In contrast the quadrature PLDMR component retains its sign within the same experimental frequency range. We account for these peculiar dynamics by a model in which the polaron recombination is spin dependent (SDR). Specifically by solving the SDR rate equations we found that it correctly explains the PLDMR frequency dependent phase, and reproduce the obtained increase of $f_0$ vs. applied voltage for single layer organic light emitting devices (OLEDs) have been investigated. The electron trap densities increased with the increase of...
Thursday, March 8, 2007 11:15AM - 2:15PM —
Session V27’DMP DCOMP: Focus Session: Computational Nanoscience VIII - Nanotransport, Contact and Conduction
Colorado Convention Center 301

11:15AM V27.00001 Understanding Molecular Conduction: Old Wine in a New Bottle?1, AVIK GHOSH, Dept. of Electrical and Computer Engineering, University of Virginia — Molecules provide an opportunity to test our understanding of fundamental non-equilibrium transport processes, as well as explore new device possibilities. We have developed a unified approach to nanoscale conduction, coupling bandstructure and electrostatics of the channel and contacts with a quantum kinetic theory of current flow. This allows us to describe molecular conduction at various levels of detail, from quantum corrected compact models, to semi-empirical models for quick physical insights, and ‘first-principles’ calculations of current-voltage (I-V) characteristics with no adjustable parameters. Using this suite of tools, we can quantitatively explain various experimental I-Vs, including complex reconstructed silicon substrates. We find that conduction in most molecules is contact dominated, and limited by fundamental electrostatic and thermodynamic restrictions quite analogous to those faced by the silicon industry, barring a few interesting exceptions. The distinction between molecular and silicon electronics must therefore be probed at a more fundamental level. Ultra-short molecules are unique in that they possess large Coulomb energies as well as anomalous vibronic couplings with current flow — in other words, strong non-equilibrium electron-electron and electron-phonon correlations. These effects yield prominent experimental signatures, but require a completely different modeling approach — in fact, popular approaches to include correlation typically do not work for non-equilibrium. Molecules exhibit rich physics, including the ability to function both as weakly interacting current conduits (quantum wires) as well as strongly correlated charge storage centers (quantum dots). Theoretical treatment of the intermediate coupling regime is particularly challenging, with a large ‘fine structure constant’ for transport that negates orthodox theories of Coulomb blockade and phonon-assisted tunneling. It is in this regime that the scientific and technological merits of molecular conductors may need to be explored. For instance, the tunable quantum coupling of current flow in silicon transistors with engineered molecular scatterers could lead to devices that operate on completely novel principles.

1Acknowledgements: DARPA, ARO, SBC, NCN, INAC

11:51AM V27.00002 Ab initio Green’s function method and Boltzmann averaging for electrical conductance of a single molecular junction, TOMOFUMI TADA, ARIHIRO TAWARA, TOSHIYA MATSUYAMA, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo, CREST-JST, SATORU TANIBAYASHI, HIDEO SEKINO, Department of Knowledge-Based Information Engineering, Toyoohashi University of Technology — The electrical conductance through benzene-dithiolate (BDT) between gold electrodes has been studied by a new approach. The Au electrodes are modeled by 3-layer (111) films and the self-assembled monolayer (SAM) of Au-benzene-1,4-dithiol- S, and then examined the interface structures, electronic states and electric properties of the Ag-Ag S-Ag system, using the non-equilibrium electron distribution function is approximated by the Fermi-Dirac distribution function with a position dependent chemical potential to reflect spatial variation of the local electrostatic potential. The electronic states of the whole Au-film-SAM-Au film system are calculated and are regarded as standing waves, which can be decomposed into +z and –z moving waves, Ψ+ and Ψ− respectively, where z is the coordinate normal to the electrodes. The current per molecule is obtained from the standard quantum mechanical current densities of the Ψ+ and Ψ− states. With this approach the calculated I-V characteristic is improved substantially with respect to those obtained by the conventional transmission-probability-Green-function type approaches.

This work was supported by the National Science Council of Taiwan. (Contract number: NSC 94-2112-M-110-012)

12:03PM V27.00003 The current-voltage characteristic of a metal-molecule-metal junction studied by an integrated and piecewise thermal equilibrium approach1, Y.-H TANG, T.-H LU, M.-H TSAI, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan — The current-voltage characteristic of a metal-molecule-metal junction has been studied by a new approach. The Au electrodes are modeled by 3-layer (111) films and the self-assembled monolayer (SAM) of Au-benzene-1,4-dithiol molecule-Au molecules is sandwiched between them. The non-equilibrium electron distribution function is approximated by the Fermi-Dirac distribution function with a position dependent chemical potential to reflect spatial variation of the local electrostatic potential. The electronic states of the whole Au-film-SAM-Au film system are calculated and are regarded as standing waves, which can be decomposed into +z and –z moving waves, Ψ+ and Ψ− respectively, where z is the coordinate normal to the electrodes. The current per molecule is obtained from the standard quantum mechanical current densities of the Ψ+ and Ψ− states. With this approach the calculated I-V characteristic is improved substantially with respect to those obtained by the conventional transmission-probability-Green-function type approaches.

This work was supported by the National Science Council of Taiwan. (Contract number: NSC 94-2112-M-110-012)

12:15PM V27.00004 First-Principles Investigation on Atomic and Electronic Transport in Ag-AgS-Ag, ZHONGCHANG WANG, TAKUYA KADOHIRA, TOMOFUMI TADA, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo and CREST-JST — A novel atomic switch using Ag-AgS-Ag heterostructure has seized a wide range of attentions recently. Its switching mechanism, however, has not been understood sufficiently. As a first step to clarify the mechanism, we investigated migration pathways of Ag ions and activation energies for the migration in Ag-S, and then examined the interface structures, electronic states and electric properties of the Ag-AgS-Ag system, using the density functional theory. The calculated activation energies for the migration are between 0.31 to 0.50 eV, which are comparable to the experimental values of 0.43 to 0.48 eV. The calculated transmission coefficient of Ag-AgS-Ag at the Fermi level increases from 0.04 before atomic relaxation to 0.455 after relaxation, which shows the opening of a conduction channel in the relaxed structure. Further analysis of atomic configuration in the relaxed structure shows formation of a chain-like arrangement of Ag in AgS.

12:27PM V27.00005 GW electronic Correlations in Quantum Transport : Renormalization and finite lifetime effects on real systems, PIERRE DARANCET, LEPES-CNRS and Université Joseph Fourier, Grenoble, ANDREA FERRETTI, Dipartimento di Fisica, Università di Modena e Reggio Emilia, and INFN-CNRS-S3, National Center on nanoStructures and bioSystems at Surfaces, 41100, DIDIER MAYOU, VALERIO OLEVANO, LEPES-CNRS — We present an ab initio approach to electronic transport in nanoscale systems which includes electronic correlations through the GW approximation. With respect to Landauer approaches based on density-functional theory (DFT), we introduce a physical quasiparticle electronic-structure into a non-equilibrium Green’s function theory framework. We use an equilibrium non-selfconsistent O(11t) self-energy considering both full non-hermiticity and dynamical effects. The method is applied to a real system, a gold mono-atomic chain. With respect to DFT results, the conductance profile is modified and reduced by the introduction of diffusion and loss-of-coherence effects. The linear response conductance characteristic appear to be in agreement with experimental results.
12:39PM V27.00006 Non-equilibrium Transport in Carbon based Adsorbate Systems. JOACHIM FÜRST, Atomistic A/S and MIC, DTU, MADS BRANDBYGE, MIC, DTU, KURT STOKBRO, Atomistix.com, ANTTI-PEKKA JAUNO, MIC, DTU — We have used the Atomistix Tool Kit (ATK) and TranSIESTA[1] packages to investigate adsorption of iron atoms on a graphene sheet. The technique of both codes is based on density functional theory using local basis sets[2], and non-equilibrium Green’s functions (NEGF) to calculate the charge distribution under external bias. Spin dependent electronic structure calculations are performed for different iron coverages. These reveal adsorption site dependent charge transfer from iron to graphene leading to screening effects. Transport calculations show spin dependent scattering of the transmission which is analysed obtaining the transmission eigenchannels for each spin type. The phenomena of electromigration of iron in these systems at finite bias will be discussed, estimating the so-called wind force from the reflection[3].

1:03PM V27.00008 Atomic dimer shuttling and two-level conductance fluctuations in Nb nanowires1, ROBERT N. BARNETT, CHUN ZHANG, ALEXEI MARCHENKOV, ZHENTING DAI, UZI LANDMAN, School of Physics, Georgia Institute of Technology — We describe density-functional structural optimization and conductance calculations which were carried out to explain high-resolution conductance measurements of niobium nanowires. In particular, the observed bistability manifesting itself as telegraph noise in the measured conductance is associated with the formation of a niobium dimer between the opposing electrodes, with the dimer shuttling between symmetric, high-conductance, and asymmetric, low-conductance, configurations.

1Supported by DOE and NSF (RNB, CZ, and UL), and by NSF and GaTech through NNRP (AM and ZD). Calculations were performed at the Center for Computational Materials Science at GaTech and at NERSC.

1:15PM V27.00009 Electronic Structure of Metal-Semiconductor Nanocontacts1, DENIS DEMCHENKO, LIN-WANG WANG, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Future nanoelectronics will depend on the electron/hole transport in a nanostructure and across nanostructure/metal electrode interfaces. Measurements of nanoscale transport are often conducted by contacting a semiconductor nanostructure with large metallic electrodes. Theoretical interpretation of such experiments, however, is often based on electronic structure of an isolated nanostructure, ignoring the influence of the electrodes. Here we address this issue by calculating the classical electrostatic polarization potential \( P(r) \), and incorporating it into the atomistic pseudopotential method, to calculate the electronic structure of experimentally-relevant sizes of nanorods. We calculate several electron/niobium dimer configurations with varying contact depths. We show that the presence of an electrode can produce localized electron and hole states near the electrode. The localization is caused by the spatial variation of the \( P(r) \). We have calculated the effects of the applied bias necessary to overcome the electron/hole localization, as well as the change of the band gap and the binding energy of the localized state as functions of the nanorod-electrode separation.


1:27PM V27.00010 Benchmark Quantum Monte Carlo Calculations of Optical gaps of carbon Nanotubes, FERNANDO REBOREDO, PAUL KENT, Oak Ridge National Laboratory — Optical properties of single wall carbon nanotubes SWCNT have attracted considerable experimental and theoretical attention because they are strongly dependent on the details of the atomic structure (chiral vector). In these systems electronic correlations have been shown to play a dominant role both theoretically [1] and experimentally [2] as electron-electron interactions are increased in low dimensions. In this talk we present ongoing calculations of the optical gaps and quasi-particle energies of SWCNT with an alternative ab-initio technique: Diffusion Quantum Monte Carlo (DMC). We take advantage of a novel algorithm based on non-orthogonal localized orbitals that allows almost linear scaling calculations for ~1000 electrons. DMC is a complementary technique to methods based on the GW approximation and the Bethe-Salpeter equation avoiding strong approximations. While the full absorption spectra cannot be obtained with DMC, we provide accurate benchmark values for the quasiparticle energy gaps and exciton binding energies. Research sponsored by the Division of Materials Sciences and Engineering, U. S. DOE; under Contract DE-AC05-00OR22725 with UT-Battelle, LLC. and by the Division of Scientific User Facilities, U. S. DOE. This work used resources of the NCCS at ORNL.


1:39PM V27.00011 First-principles study of effects of metallic electrode contacts on transport properties of carbon nanotubes, NOBUHIKO KOBYASHI, Inst Appl Phys, Univ Tsukuba, Japan, TAISUKE OZAKI, Res Inst Comp Sci, AIST, Japan, KENJI HIROSE, Fund Env Res Lab, NEC, Japan — Towards a development of constructing nanometer-scale devices, considerable effort has been made in experiments using carbon nanotubes for fabricating nanoscale field-effect transistors. To detect electric signals, electrodes must be connected to the conductors. Contact with the electrodes sensitively influences the transport properties. Therefore, we have studied the transport properties on the basis of the detailed electronic state calculation that includes the effect of contact with the electrodes. We have investigated quantum transport in carbon nanotubes bridged between metallic electrodes. The electronic states are calculated using a numerical atomic orbital basis set in the framework of the density functional theory, and the conductance is calculated using the Green’s function method. We have analyzed transport properties of the finite size of carbon nanotubes bridged between Al, Au, Pt, Pd metallic electrodes, and discuss the contact effect of the electrodes on the transport properties. We reveal their dependency on the electrode materials.
1:51PM V27.00012 Nano-helix based quantum transistor, charge pump and motor. XIOLIANG QI, SHOUCHENG ZHANG, Stanford University — We propose several novel device concepts based on nano-scale carbon nanotubes (SWNTs). Applying a static electric field transverse to the helical wire induces a metal to insulator transition, enabling the construction of a new type of transistor switch. The band gap is purely determined by the applied transverse voltage, and can be continuously tuned. The resulting light-emitting diode can emit light with a tunable color spectrum. With a quadrupolar electrode configuration, the electric field could rotate in the transverse plane, leading to a quantized dc charge current proportional to the frequency of the rotation. Such a device could be used as a new standard for the high precision measurement of the electric current. The inverse effect implies that passing an electric current through the helical wire in the presence of a transverse static electric field leads to a mechanical rotation of the helix. This effect can be used to construct nano-scale electro-mechanical motors. Finally, our methodology also enables new ways of controlling and measuring the electronic properties of helical biological molecules such as the DNA.

2:03PM V27.00013 Low temperature transport properties of semiconducting nanocrystal arrays. ANDREAS GLATZ, IGOR BELOBORODOV, VALERII VINOKUR, Argonne National Lab — We study the electron transport in semiconducting nanocrystal arrays at temperatures $T ≪ E_c$, where $E_c$ is the charging energy for a single grain. In this temperature range the electron transport is dominated by co-tunneling processes. We discuss both elastic and inelastic co-tunneling and show that for semiconducting nanocrystal arrays the inelastic contribution is strongly suppressed at low temperatures. We also compare our results with available experimental data.

Thursday, March 8, 2007 11:15AM - 2:15PM —
Session V28 DMP: Focus Session: Carbon Nanotubes: Chemistry Colorado Convention Center 302

11:15AM V28.00001 Resonance Raman spectroscopy of length fractionated single-walled carbon nanotubes1. A. HIGHT WALKER, J.A. FAGAN, B.J. BAUER, E.K. HOBBIE, J.R. SIMPSON, National Institute of Standards and Technology, Gaithersburg, MD 20899 — In many potential applications of single-walled carbon nanotubes (SWNTs), the difficulty of separating nanotubes by their structural properties, e.g., length and chirality, remains an impediment to their widespread implementation. Our studies include HiPco, CoMoCat, and arc-discharge SWNTs wrapped with 30-mer 5'-GT(GT)13-3' single-stranded DNA and dispersed in solution. These samples display an exceptionally low degree of SWNT bundling and clustering, in the limit of nanodispersion. Size-exclusion chromatography collects length fractions ranging in size from < 100 nm to ~ 400 nm. Multi-angle light scattering, AFM, and TEM characterize the length distribution of each fraction. We measure resonance Raman spectroscopy (RRS) over a wide range of laser excitation wavelengths for vibrational modes including the radial breathing mode (RBM) and higher order graphite modes. All modes exhibit a monotonic increase of Raman scattering intensity with increasing nanotube length. We discuss these results in terms of an optical scattering model. Furthermore, we hybridize these length separated fractions with complimentary DNA sequences functionalized with nanoparticles to study the effects of DNA-wrapping on SWNT properties.

1Work supported by NIST-NRC postdoctoral fellowship.


11:27AM V28.00002 Modeling of the SWNT-DNA complexes in the water solution. ALEXEY A. TSUKANOV, EUGENE A. GRACHEV, Moscow State University, SLAVA V. ROTKIN, Physics Department and Center for Advanced Materials and Nanotechnology, Lehigh University — It is known that the single-wall nanotubes (SWNTs) may form a hybrid with a single-stranded DNA having a regular helical structure of the DNA wrap around the SWNT cylinder. Such DNA wrapping creates a periodic potential at the NT surface, which results in developing structure symmetry-lowering effects may result in variation of the optical spectra, especially for (slightly forbidden) transverse optical transitions. The effect of environmental screening of charges is investigated. Self-consistent electrostatic calculations yield cohesion energy between a charged, regular wrap and a solvent and provide heuristic physics interpretation of the results. We show that the NT screening is different from what one expects for a metal or insulator material due to non-local Coulomb correlations. An effective dielectric screening of the water exterior is extracted from the simulations.

11:39AM V28.00003 Electronic structure of single-walled carbon nanotubes inside helical DNA wraps. STACY SNYDER, SLAVA ROTKIN, Lehigh University — Single stranded DNA can helically wrap a single-walled carbon nanotube (SWNT) leading to changes in electronic structure, which is the subject of our study. Other charged polymers may produce band gap modulation similar to that observed for DNA-SWNT complexes. For these hybrids we assume a regular helical wrap, the potential of which breaks the symmetry of the pristine SWNT. Band structure changes are modeled quantum mechanically using the tight binding method together with self-consistent electrostatics. Gap modulation and band structure symmetry-lowering effects may result in variation of the optical spectra, especially for (slightly forbidden) transverse optical transitions. The effect of environmental screening of charges is investigated. Self-consistent electrostatic calculations yield cohesion energy between a charged, regular wrap and a SWNT of the order of tenths of eV per DNA base [1]. [1] Snyder, S. E., and Rotkin, S. V., Polarization Component of Cohesion Energy in Single-Wall Carbon Nanotube-DNA Complexes, JETP Letters 84, 348 (2006).

11:51AM V28.00004 Aminoacid Functionalization and Raman Characterization of DWNT. MORENO MENEGHETTI, GABRIELE MARCOLONGO, GIORGIO RUARO, VINCENZO AMENDOLA, JESSICA ALFONSI, MARINA GOBBO, University of Padova, Dep. Chemical Sciences — Carbon nanotubes are difficult to manipulate because of their aggregation and low reactivity. For this reason many types of functionalization have been obtained and, usually, large functionalizations are needed. However, in particular considering single wall carbon nanotubes (SWNT), a large functionalization modifies the electronic properties because it introduces a large number of defects states. To overcome this problem we have considered double wall carbon nanotubes (DWNT) which can be considered as SWNT protected by an external carbon nanotube. We have performed an oxidation and a functionalization of DWNT covalently linked charged aminoacids. From the Raman characterization of the functionalized nanotubes we find that the external nanotubes have been modified by the functionalization but not the internal ones. We think that this is an interesting approach to obtain carbon nanotubes which are easy to manipulate but with electronic properties, in this case of the internal nanotube, which are preserved.
12:03PM V28.00005 Directed Linking of Carbon Nanotubes with CdSe Quantum Dots and Au Nanoparticles. KATHRYN LEACH, TODD KRAUSS, University of Rochester — As circuit miniaturization continues, the demand for smaller and more efficient component parts has increased. Metallic single-walled carbon nanotubes (SWNTs) are the ideal nanometer-scale wire, as they can withstand current densities up to 2 to 3 orders of magnitude higher than copper currently used in electronic chips. These conductive nanotubes can therefore be utilized as “nano-electrodes” to efficiently electrically connect another nanoscale object, such as a single semiconductor quantum dot (QD) or metallic nanoparticle (NP), thus creating macroscopic integrated systems based on nanometer-scale components. Although NPs have been previously attached to NTS, the attachment scheme was uncontrolled; direct and defined attachment of NPs to SWNTs remains elusive. We have designed a strategy for directed assembly of fabricated QD–SWNTs. NTs were grown across patterned catalyst islands on a silicon wafer followed by electrode placement. After cutting the NTS, the resulting carboxylic group moieties found at the cut NT edges were used to covalently attach CdSe QDs or Au NPs. Electrostatic force microscopy (EFM) and transport measurements were used to monitor NT conductivity before and after cutting, as well as after NP attachment. The photoelectrical transport properties of a typical hybrid QD–SWNT device will be discussed.

12:15PM V28.00006 Size Selective Interaction of Single Wall Carbon Nanotubes with Collagen. SANJIB BHATTACHARYYA, JEAN-PAUL SALVETAT, CRMD-CNRS, 1B rue de la Ferollerie, Orleans 45071, France, DEBDULAL ROY, National Physical Laboratory, Hampton Road, Teddington, Middlesex TW11 0LW, U.K., MARIE-LOUISE SABOUNGI, CRMD-CNRS, 1B rue de la Ferollerie, Orleans 45071, France — One of the big challenges in using single-wall carbon nanotubes (SWNTs) in nanotubeelectronics at the present time is to produce SWNT’s of specific diameters. Unfortunately, it is almost impossible to achieve this by existing synthesis procedures. All these produce SWNT’s with a mixture of diameters and chiralities and, therefore, different electrical properties such as semiconducting and metallic. Here, we propose a method of functionalization that selects SWNTs of a single specific diameter from a mixture of tubes. We have shown that denaturation of collagen type-I solution in the presence of sodium dodecyl sulphate (SDS) and SWNT’s leads to wrapping of carbon nanotubes of a specific diameter by collagen peptides, which are soluble in water. Separation is achieved by centrifugation of the solution at 10,000 RPM and taking the supernatant, which is rich in nanotubes having one specific diameter.

12:27PM V28.00007 Optical modulation of single walled carbon nanotubes. MICHAEL S. STRANO, University of Illinois at Urbana-Champaign — Recent advances in the spectroscopy of single walled carbon nanotubes have significantly enhanced our ability to understand and control their surface chemistry, both covalently and non-covalently. Our work has focused on modulating the optical properties of semiconducting single walled carbon nanotubes as near infrared photoluminescent sensors for chemical analysis. Molecular detection using near-infrared light between 0.9 and 1.3 eV has important biomedical applications because of greater tissue penetration and reduced auto-fluorescent background in thick tissue or whole-blood media. In one system, the transition of DNA secondary structure modulates the dielectric environment of the single-walled carbon nanotube (SWNT) around which it is adsorbed. The SWNT band-gap fluorescence undergoes a red shift when an encapsulating 30-nucleotide oligomer is exposed to counter ions that screen the charged backbone. We demonstrate the detection of the mercuric ions in whole blood, tissue, and from within living mammalian cells using this technology. Similar results are obtained for DNA hybridization and the detection of single nucleotide polymorphism. We also report the synthesis and successful testing of near-infrared β-D-glucose sensors that utilize a different mechanism: a photoluminescence modulation via charge transfer. The results demonstrate new opportunities for nanoparticle optical sensors that operate in strongly absorbing media of relevance to medicine or biology.

1:03PM V28.00008 Targeted Damage of Carbon Nanotubes. LUKE DONEV, PAUL MCEUEN, Laboratory of Atomic and Solid-State Physics, Cornell University — One possible pathway to fabricating a narrow strip of graphene would be to cut open a carbon nanotube. To that end, we have explored a procedure for selectively damaging carbon nanotubes. Nanotubes of diameter 3-10 nm were grown from iron nanoparticles and electrical contacts were lithographically applied to make transistor devices several microns long. To selectively damage the nanotubes a region was opened in a blanket of photoresist over the tube. A thin aluminum oxide layer (2-3 nm) was deposited at an angle in the exposed region to partially protect the nanotube. The nanotubes were then briefly exposed to an oxygen plasma. After the plasma etch and removal of the photoresist and aluminum oxide, a fraction of the nanotubes no longer conduct and others have higher resistance. For some of the nanotubes with increased resistance there is a height difference between the damaged and undamaged sections and scanned gate microscopy shows enhanced sensitivity in the etched region.

1:15PM V28.00009 Ab Initio Study of Crosslinking of Functionalized Carbon Nanotubes1. IGOR VASILEV, SEAMUS A. CURRAN, Department of Physics, New Mexico State University — We investigate the mechanism of covalent crosslinking between carbon nanotubes functionalized with thiocarboxylic and dithiocarboxylic esters. The structures of interconnected nanotubes are modeled in the framework of density functional theory combined with the pseudopotential approximation. Our calculations reveal an important role of surface defects in the formation of chemical bonds connecting nanotubes to each other. The strength and stability of intertube bonds increases in the vicinity of defect sites. The computed binding energies and potential energy profiles of linked nanotubes are found to be sensitive to the choice of the exchange-correlation functional used within the density functional formalism. This sensitivity could be explained by a nonuniform distribution of the electronic charge density near defect sites. Our results imply that the use of gradient-corrected functionals is essential for accurate theoretical modeling of functionalized carbon nanotubes and nanotube-based composites.

1Supported by NSF DMR-0505270, PRF 43409-G10, and AFOSR FA-9550-05-1-0234.

1:27PM V28.00010 Deformation of sp2 graphitic nanostructure by irradiation with highly charged ion1. YOSHIYUKI MIYAMOTO, Fundamental and Environmental Research Laboratories, NEC — I will discuss possibility of structural deformation of graphitic sp2 network by irradiation of highly charged ions. Meguro et al., [Appl. Phys. Lett. 79, 3866 (2001)] reported indication of nano-diamond formation on graphite surface when it is irradiated by Ar+8 ions with incident kinetic energy of 400 eV. The nano-diamond structure was suggested from STS and IR spectrum taken after irradiation showing energy gap of 6 eV and C-C stretching with the frequency of 1360 cm-1. This structural change was considered to be induced by injection of holes from highly charged ion (Ar+8) while role the kinetic energy of Ar ion was thought to be marginal. Electron-ion dynamics simulation combined to the time-dependent density functional theory [O. Sugino, Y. Miyamoto. Phys Rev B59, 2579 (1999), ibid. Phys. Rev. B66, 085901(E) (2002)] has been performed to examine the mechanisms of the structural change. This simulation has found that the role of incident kinetic energy of Ar+8 and subsequent cooling mechanisms also play crucial role in determining the structural change. More details will be presented and discussed in my talk.

1All calculations were performed by using the Earth Simulator.

1:39PM V28.00011 Metallic carbon nanotubes destruction using Laser Irradiation. HISASHI KAJIURA, HOIJIN HUANG, RYUCHIRO MARUYAMA, KOJI KADONO, KAZUHIRO NODA, Sony Corporation — We demonstrated that, using laser irradiation in air, metallic single-walled carbon nanotubes (SWNTs) in carbon nanotube thin film can be preferentially destroyed to their semiconducting counterparts if SWNTs are not heavily bundled. Although all metallic SWNTs were not destroyed using the lasers with an excitation wavelength of 514.5nm and 632.8nm due to a large distribution of SWNT diameters, it is clear that if SWNTs with a small distribution of diameter can be produced, it should be possible to destroy all of the metallic SWNTs using one or two lasers. [Huang et al. J.Phys.Chem.B, 2006, 110, 7316-20. and 4686-90]
11:15AM V31.00001 Thermoelectric power of Single Walled Carbon Nanotubes at the Ballistic Conduction Limit . YURI M. ZUEV, Applied Physics Department, Columbia University, PHILIP KIM, Physics Department, Columbia University — Thermoelectric power (TEP) measurements of single walled carbon nanotubes(SWNTs) with low electrical contact resistance are reported. TEP was measured in-situ using a microfabricated heater and thermometers. High quality Ohmic contact to the SWNT was achieved with Pd electrodes. TEP measurements are sensitive to the change in conductivity, and therefore provide a complementary method for probing the electronic band structure of SWNTs. Deviations of the low temperature TEP gate dependence from the semiclassical Mott relation allows us to gain insight into the quantum transport regime in this one dimensional conductor. Modulation of TEP as a function of applied gate voltage will be discussed in connection with the shell filling effects and Fabri-Perot oscillations observed in electrical conductance.

11:27AM V31.00002 Phonon-Phonon Interaction In Carbon Nanotube Assemblies. ALI ALIEV, MEI ZHANG, ANVAR ZAKHIDOV, RAY BAUGHMAN, Nanotech Institute, University of Taxes at Dallas, Richardson, TX 75083 — We present the comparative study of the anisotropic 1D thermal conductivity and the thermal diffusivity of assemblies of carbon nanotubes (CNTs) comprising an increasing number of aligned free standing carbon nanotubes (SWNT and MWNT) using two techniques: laser flash and self-heating 3u methods. The concept of mode quenching is considered for alignment of few individual CNTs. The length dependence of thermal conductivity is studied for CNT with different number of intrinsic defects (HiPCO, Laser ablation, Arc-Charge). The extremely high surface area of CNT assemblies like highly aligned MWNT sheet [1] leads to the excessive radial radiation of the heat and dose not allow to transfer the heat energy by means of phonons to distances more than 2 mm. [1]. M. Zhang, S. Fang, A. A. Zakhidov, S. B. Lee, A. E. Aliev, C. D. Williams, K. R. Atkinson, R. H. Baughman, Science 309, 1215 (2005).

11:39AM V31.00003 Electromechanical Resonators from Atomically Thin Graphite. SCOTT BUNCH, AREND VAN DER ZANDE, SCOTT VERBRIDGE, Cornell Center for Materials Research, IAN FRANK, DAVID TANENBAUM, Pomona College, JEEVAK PARPIA, HAROLD CRAIGHEAD, PAUL MCEUEN, Cornell Center for Materials Research — We fabricate nanoelectromechanical systems (NEMS) from atomically thin graphite by mechanically exfoliating thin sheets over trenches in SiO2. Vibrations with fundamental resonant frequencies in the MHz range are actuated either optically or electrically and detected optically by interferometry. We make a detailed study of the mechanical properties of these resonators including resonance frequency, spring constant, built in tension, and quality factor. The thinnest resonator consists of a single suspended layer of atoms and represents the ultimate limit of a two dimensional NEMS.

11:51AM V31.00004 Microwave Nano-abacus Electro-mechanical Oscillator. HAIIBING PENG, C.W. CHANG, S. ALONI, T.D. YUZVINSKY, A. ZETTL, UC Berkeley — We describe nanoscale electromechanical oscillators capable of operating in ambient-pressure air at room temperature with unprecedented fundamental resonance frequency of ~4 GHz. The devices, created from suspended carbon nanotubes loaded abacus-style with inertial metal clamps yielding short effective beam lengths, open windows for immediate practical microwave frequency nanoelectromechanical systems (NEMS) applications.

12:03PM V31.00005 Metal-carbon nanotube composite nanoelectromechanical torsional resonators. YOUNG DUCK KIM, SELING SAE HONG, JUNG HOON BAK, BYUNG YANG LEE, SUNG WOON CHO, KI SUNG SUH, SEUNGHUN HONG, YUN DANIEL PARK, Department of Physics and Astronomy, Seoul National University NS50, Seoul 151-747, Korea — Metallic based nanoelectromechanical systems (NEMS) resonator structures are of interest due to higher optical reflectivity, ductility, and conductivity compared to insulator- and semiconductor-based NEMS structures. We present NEMS torsional resonator structures fabricated from aluminum-carbon nanotube (CNT) and palladium-CNT composites. Metal and metal-CNT NEMS structures are released from III-V based substrates. The resonators are electrostatically driven and are detected at room temperatures under moderate vacuum conditions using optical modulation techniques. We note significant differences in the resonant frequencies (f0) and the quality factors (Q) between metal and metal-CNT NEMS torsional resonators. Aluminum based structures with paddle dimensions of ~5 micron x ~5 micron, with support beams of ~1 micron x ~3 micron, show a fundamental resonant frequency corresponding to translational mode of 1.7 MHz with Q of 20, while Al-CNT based structures of same dimensions show f0 of 3 MHz and Q of 50, as a typical example. We will further discuss the effects on the mechanical properties of metallic NEMS torsional resonators due to addition of CNT.
12:15PM V31.00006 Negative Differential Friction in Sliding Nanotubes, UGO TARTAGLINO, Democritos National Simulation Center and SISSA, Trieste, Italy, XIAO-HUA ZHANG, Surface Physics Laboratory and Department of Physics, Fudan University, Shanghai, China, GIUSEPPE E. SANTORO, International School for Advanced Studies (SISSA), and Democritos National Simulation Center, Trieste, Italy — Sliding friction is often simulated by moving sliders at some externally imposed relative velocity \( v \), and calculating the resulting friction force \( f \). However this is at variance with experimental results in real life, where the force \( f \) is applied, and a sliding velocity \( \dot{v} \) results. We report that in some cases the force is monotonic the two procedures are equivalent, but when it is nonmonotonic, it is not. In the realistic case of an applied force one may expect characteristic velocity instabilities, due to regions of “negative differential friction,” where \( \frac{df}{d\dot{v}} < 0 \). We exemplify this phenomenon for the case of two single walled nanotubes sliding inside one another. The sliding velocity is predicted to exhibit striking plateaus and jumps as the pulling force increases.

12:27PM V31.00007 Status sensitivity in the photocurrent of single wall nanotubes, PRASANTH GOPINATH, A. MOHITE, H. SHAH, J. LIN, B. NAGABHIRAVA, T. BANSAL, B. ALPHENAAR, University of Louisville — The energy spectrum of carbon nanotubes is highly sensitive to strain and mechanical deformation. Calculations predict a shift in the bandgap of single wall nanotubes (SWNT) with axial strain, which in turn affects the conductance. We have measured the influence of strain on the photocurrent spectrum of SWNT’s and observe as much as 600meV shift in the band gap energy of semiconducting nanotubes for 300 micro strains. The experiments were performed on SWNT’s CVD grown on a 300μm thick quartz cantilever; the SWNT’s are strained by pushing down on the free end of the cantilever. We use a capacitive photocurrent technique for detecting the photocurrent as a function of incident photon energy. The peak corresponding to the band- to- band free electron transition in the semiconducting nanotubes is observed to shift to lower energies with increasing strain. Further measurements using a fixed wavelength (488nm) Ar ion laser show as much as an order of magnitude change in the photocurrent with strain, implying a gauge factor of more than a 1000. Our measurements provide a direct probe of the influence of strain on the bandgap of SWNT’s and open up the possibility of using SWNT’s as optical strain sensors.

12:39PM V31.00008 Nanotubes stretched in Liquid-Metal-Ion-Sources:their influence on the cluster emission and on the isotopic anomalies, RENE JEAN TARENTO, PIERRE JOYES, JEAN VAN DE WALLE, LPS universite de Paris Sud — The present contribution argues that an intense electric field (few V/A) provides an alternative method to stretch matter and to form nanotubes locally. The very high electric field is supplied by a Liquid Metal Ion Source (LMIS). Intriguing aspects are displayed by the LMIS mass spectra of some pure elements. The periodicity of pure Ge or Sn LMIS i.e. series of equidistant peaks such Ge\(_{6n+1}\) with \( n = 3 \) to 8 or Ge\(_{6n+4}\) with \( n = 7 \) to 14 or the formation of unexplained Au\(_{8}^{4+}\) and Au\(_{10}^{6+}\) ions for the pure Au LMIS are attributed to the existence of Ge, Sn or Au nanotubes in operating LMIS. LMIS results on eutectic Au\(_{73}^{1+}\)Ge\(_{27}\) alloy show the formation of a gold nanotube associated with the strong Au\(_{8}^{4+}\) emission. The Ge\(_{27}\) emitted near the gold nanotube interact with a larger electric field than in the pure Ge LMIS provoking a bond break in hetero-isotope dimers and therefore isotope anomalies in dimer emission. Finally we analyse the results from Au-Si eutectic.

12:51PM V31.00009 Organic-vapor-induced repeatable movements of C\(_{60}\) in/from single-wall carbon nanohorns at room temperature, JIN MIYAWAKI, JST/SORST, MASAKO YUDASAKA, JST/SORST and NEC, RYOTA YUGE, NEC, SUMIO IIJIMA, JST/SORST, NEC, and Meijo Univ. — Incorporation of functional materials inside carbon nanotubes (CNTs) has been actively investigated with the goal of improving the physical and chemical properties of CNTs. We found intriguing phenomena of repeatable movement of materials from inside to outside of CNTs and vice versa, which resulted simply by exposure to different organic vapors at room temperature. For example, C\(_{60}\) entered inside single-wall carbon nanohorns (SWNHs), a type of single-wall CNTs, when exposed to toluene vapor at room temperature, and the incorporated-C\(_{60}\) exited when exposed to ethanol vapor. Here the entrance and exit were evidenced by X-ray diffraction and N\(_2\) adsorption measurements, and microscopic observations. The back-and-forth transportations of C\(_{60}\) could be repeated. We think that the C\(_{60}\) movements were mediated by the layers of toluene or ethanol adsorbed on the SWNH surfaces. The present findings will help in the fabrication of various nanometer-scale hybrid systems from CNTs.

1:03PM V31.00010 Resonance Raman study of polyyne inside single-walled carbon nanotubes, MARCOS PIMENTA, LEANDRO MALARD, Departamento de Fisica, Universidade Federal de Minas Gerais, DAISUKE NISHIDE, Department of Chemistry, Nagoya University, ANA PAULA GOMES, ADO JORIO, Departamento de Fisica, Universidade Federal de Minas Gerais, HISANORI SHINOHARA, Department of Chemistry, Nagoya University — We report a resonance Raman study of polyyne C\(_{n}\)H\(_{2}\) molecules \((n = 10 \text{ and } 12)\) composed of linearly bonded sp-carbon atoms aligned inside the single-walled carbon nanotubes (SWNTs), using many laser lines in the range 1.9 to 2.7 eV. The C10H2@SWNT hybrid material exhibits a Raman peak at 2066 cm\(^{-1}\) related with the stretching vibration of the C10H2 molecules interacting with SWNTs, while the C12H2 disrupted in n-axene exhibits peaks in the UV, around 4.9 and 4.5 eV, respectively. This result can be associated with a two-photon Raman resonance that is at variance with what happens in most cases in real life, where the force \( f \) is applied, and a sliding velocity \( \dot{v} \) results. The optical absorption spectrum of the purified C\(_{10}\)H\(_{2}\) and C\(_{12}\)H\(_{2}\)@SWNT materials, respectively. However, the optical absorption spectrum of the purified C10H2 and C12H2@SWNT materials, respectively. The peak corresponding to the band- to- band free electron transition in the semiconducting nanotubes is observed to shift to lower energies with increasing strain. Further measurements using a fixed wavelength (488nm) Ar ion laser show as much as an order of magnitude change in the photocurrent with strain, implying a gauge factor of more than a 1000. Our measurements provide a direct probe of the influence of strain on the bandgap of SWNT’s and open up the possibility of using SWNT’s as optical strain sensors.

1:15PM V31.00011 Localization of inserted species inside single walled carbon nanotubes bundles: experimental and ab initio study, NEDJMA BENDIAB, LPS-Univ J Fourier-Grenoble, A. MARCO SAITTA, IMPMC-Univ Pierre et Marie Curie-Paris 6, ROBERT ALMAIRAC, RAYMOND AZNAR, JEAN-LOUIS SAUVAJOL, LCVN-Univ Montpellier II, ISABELLE MIREBEAU, LLB-CEA Saclay — The aim of this work is to understand the structural organization of inserted alkali atoms inside single walled carbon nanotube bundles. First of all, we present X-rays and neutrons diffraction results obtained on rubidium inserted carbon nanotubes. The results of X-rays and neutrons diffraction experiments are surprising and in apparent contradiction, and will be discussed in connection with the debated question of the lattice expansion of the hexagonal tubes framework under insertion. The possible insertion sites of the rubidium atoms in the nanotube bundle will be discussed in terms of their effects on the diffraction spectra. The experimental results will be compared to diffraction simulations and ab initio DFT calculations. The main outcome of our combined experimental and theoretical study is that: i) up to saturation, the spectra show no lattice expansion; ii) the extinction of the (10) peak is only compatible with Rb insertion inside the tubes; iii) DFT calculations show that constant lattice parameter the insertion within the tubes is energetically favored with respect to insertion between the tubes.

1:27PM V31.00012 Experimental Evidence for Water Intercalation into Graphite, DINKO CHAKAROV, HANS FREDRIKSSON, GUIDO KETTELER, BENGT KASEMO, Department of Applied Physics, Chalmers University — Using different experimental methods we follow the uptake and release of water from highly oriented pyrolytic graphite sample. We found that water can intercalate into graphite following transient binding to defect sites and accumulate in the subsurface regions with concentrations amounting up to 10% of the monolayer. The process is thermally activated and could be manipulated by changing the water vapor pressure or amount of water (ice) on the surface. Photoelectron and vibration spectroscopy data indicate strong perturbation of the intercalated water molecules and lowered barrier for dissociation.
1:39PM V31.00013 Dependence of single-walled carbon nanotubes’ adsorption kinetics on temperature and binding energy

VAIVA KRUNGLEVICUTE, DINESH RAWAT, MURAT BULUT, LUKE HEROUX, ALDO MIGONE,
Southern Illinois University Carbondale — We present adsorption kinetics results for hydrogen, freon and ethane on single walled carbon nanotubes. We measured the decrease of the pressure as a function of time as equilibrium is approached. Our results indicate that the equilibration time is a function of $\frac{1}{T}$, where $T$ is the isotherm temperature and $T$ is the isotherm temperature. We also compare the dependence of the equilibration time on the shape of the adsorbate. We found that for linear molecules the equilibration times decrease with increasing coverage at a much slower rate than those times for spherical molecules.

1:51PM V31.00014 Temperature and Pressure Dependence of Hydrogen Coverage on Single-Walled Carbon Nanotubes

JUN NI, XIAOBAO YANG, Department of Physics, Tsinghua University — The safe and compact storage of hydrogen is of great interest in theoretical and experimental research. Carbon nanotubes are reported to be highly efficient for gas and alkali atom storage. The process of hydrogen adsorption on the carbon nanotubes is changed under various circumstances. It is important to know how the hydrogen coverage depends on the tube diameters, temperature and pressure. We have investigated the stability of various hydrogenated single-walled carbon nanotubes. We find the storage capacity of hydrogen depends significantly on the diameters of carbon nanotubes. The full hydrogen coverage can be reached for the nanotubes with small size, while for the nanotubes with large size, the saturation coverage is lower than $1$. We have calculated the variation of the hydrogen coverage with the change of temperature and pressure. In particular, we find that the nanotubes with diameters of about $1$ nm can achieve the coverage of $80\%$ at ambient temperature and low pressure, which is in agreement with the experimental results.

This research was supported by the National Natural Science Foundation of China under Grant No. 10474049

2:03PM V31.00015 Transport characteristics of a single multiwall carbon nanotube by bending in SEM and STM

SUENNE KIM, Materials Science & Engineering, University of Texas at Austin; JEEHOON KIM, MORGAN BERG, ALEX DE LOZANNE, Department of Physics, University of Texas at Austin — Multiwall carbon nanotubes(MWCNT’s) were grown on a W wire by chemical vapor deposition(CVD). Two homebuilt xyz-walkers were employed to manipulate individual CNTs in our scanning electron microscope (SEM). To improve the electrical and mechanical contact to a second electrode, we welded the CNT by delivering gas to the welding point while focusing the SEM beam on the same spot. The bending dependent I-V characteristics were observed in situ in the SEM at room temperature. We will measure the transport properties by bending the same MWCNT (already measured in SEM) inside our ultrahigh vacuum low temperature scanning tunneling microscope (UHV-LTSTM). We will also compare the bending properties of MWCNTs at different temperatures.

Thursday, March 8, 2007 11:15AM - 2:03PM
Session V44 DMP: Focus Session: Plasmons in Nanoholes, Arrays and Structured Surfaces
Colorado Convention Center 507

11:15AM V44.00001 Nonlinear Optical Effects in Periodic Arrays of Nanoholes in Metallic Films
XIWEN WANG, Department of Chemistry, Northwestern University; Center for Nanoscale Materials, Argonne National Laboratory, STEPHEN GRAY, Center for Nanoscale Materials, Argonne National Laboratory, GEORGE SCHATZ, Department of Chemistry, Northwestern University — Extraordinary optical transmission (EOT) by periodic subwavelength apertures in metallic films has been much studied. Recent studies have shown that different aperture shapes can give quite different transmission spectra. For circular holes, EOT is often attributed to coupling with surface plasmons. Rectangular holes, however, can show more enhanced EOT and localized modes inside the holes, as opposed to plasmons, are often the dominant features. This implies that in the process of resonant transmission, light is highly concentrated inside the holes, which opens the possibility for exploring nonlinear effects. We use the finite-difference time-domain calculations to study the transmission properties of metallic films with arrays of rectangular subwavelength holes, each hole filled with a Kerr nonlinear material. We consider both the perfect metal limit and silver that supports plasmons. We analyze the transmission spectra as a function of incident intensity. Due to the large electric fields associated with the localized modes inside the holes, moderate incoming fluxes can result in dramatic changes in the positions of the transmission peaks.

11:27AM V44.00002 Theoretical Study of Optical Transmission Enhancement through Sub-Wavelength Apertures: Determining the Role of Surface Plasmon Polaritons
PHILIP FLAMMER, JAMES MARTINEAU, REUBEN COLLINS, IAN SCHICK, MICHAEL HORIZONTZ, Colorado School of Mines, RUSSELL HOLLINGSWORTH, ITN Energy Systems, Inc. — Enhanced optical transmission (EOT) through sub-wavelength apertures in metal films has been observed from both experimental and theoretical studies of circular apertures surrounded by bulls-eye groove configurations or simpler linear apertures flanked by grooves. These studies have also generated much debate over the driving mechanisms involved. In this talk, theoretical results from a commercial finite element PDE solver will be presented with supporting experimental results for linear aperture/groove structures. This study confirms the integral role of surface plasmon polaritons in causing EOT, and also shows the importance of surface cavity resonances. Results will be presented exploring the role of the geometry of the grating structures, and how to tune the EOT resonance wavelength by changing the aperture/groove geometry. This material is based on work supported by the National Science Foundation under Grant No. DMI-052228.

11:39AM V44.00003 The coupling of surface plasmons in periodic arrays of subwavelength holes
RUWEN PENG, ZHAOHUI TANG, ZHAN WANG, YONGJUN BAO, MU WANG, National Laboratory of Solid State Microstructures, Nanjing University — We demonstrate here that transmission optical enhancement originates not only from surface plasmons(SP’s) but also from the coupling of SPs on the silver film perforated with a periodic array of subwavelength holes. We fabricate the structured silver films by coating the film with magnetron sputtering, and then drilling holes with focused-ion-beam facility. The optical measurements are in good agreement with numerical calculations based on the full-vectorial three-dimensional finite-difference time-domain method. The peaks in measured transmission spectrum have also been analytically indexed by using effective-dielectric-constant model. It is shown that the coupling of SPRs shifting from sub-wavelength transmission peaks, and increases with decreasing the thickness of silver films. We suggest that these properties open an unique way to tune electromagnetic wave in subwavelength optics.

3Supported By NSF and MOST in China.

11:51AM V44.00004 Plasmonic properties of a nanosized hole in a thin metallic film
TAE-HO PARK, PETER NORDLANDER, Department of Physics, Rice Univ. — We investigate the optical properties of a nanosize hole in a thin metallic film. We show that the optical absorption spectrum is characterized by a plasmon resonance of an energy that depends strongly on the ratio of the hole diameter and the film thickness in qualitative agreement with experimental results. Microscopically, the nanohole plasmon is shown to consist of a collective state formed by propagating thin film plasmons. The hole surface exposes the film plasmons and introduce a dipole moment which allows the coupling to incident light. We also show that the energy of the hole plasmon resonance depends strongly on the polarization and direction of the incident light.
12:03PM V44.00005 Interaction between surface plasmon and 2-dimensional nano-defects at metallic surfaces.\footnote{1} Raul Garcia-Llamas, Jorge Gaspar-Armenta, Judith Tnor-Cordova, Universidad de Sonora, Manuel Leyva-Lucero, Universidad Autonoma de Sinaloa — A theoretical study of light diffraction and intensity of near-field from two-dimensional nano-defects at metallic surface illuminated with electromagnetic plane waves is presented. Results for one or two Gaussian-shaped sub-wavelength defects at silver surface are shown. The light diffraction patterns shown minima at specific angular directions in the case of two defects separated a distance $d$. These minima are associated to the ratio $(\lambda/2d)$ and depend on the localization of the defects, being $\lambda$ the wavelength of the illumination light. The Near-Field intensity, calculated to constant height, shows oscillations associated to the excitation of surface plasmon, which amplitude are greater for smaller width of the Gaussian defect.

\footnote{1}Consejo Nacional de Ciencia y TecnologÌÁ. Proyecto 47391

12:15PM V44.00006 Mapping of the optical emission in the vicinity of the surface of a sub-wavelength aperture flanked by periodic grooves in a gold film. Ian C. Schick, James T. Martineau, Reuben T. Collins, David Flammer, Colorado School of Mines, Russell E. Hollingsworth, ITN Energy Systems, Inc — Enhanced optical transmission through subwavelength apertures surrounded by periodic features has been a subject of great recent interest. Equally important are the emission characteristics of these structures. Transmission enhancement has typically been observed as peaks in the spectral dependence of transmission measured in the far-field. Here we use near-field scanning optical microscopy to spatially map the optical emission in the vicinity of the aperture and as emission propagates into the far field. We show the dependence of the emission pattern on the wavelength of the incidence in addition to structural parameters, such as spacing between the grooved regions and the aperture and the spatial period of the grooves. We observe that the emission pattern is governed by interference effects between emission from the aperture and scattered light from adjacent surface features. This material is based on work supported by the National Science Foundation under Grant No. DMI-0522281.

12:27PM V44.00007 Dependence of Transmission Through Subwavelength Linear Apertures on Grating/Aperture Separation\footnote{1}, Michael Hurowitz, Ian Schick, Philip Flammer, James Martineau, Colorado School of Mines, Russell Hollingsworth, ITN Energy Systems, Inc, Reuben Collins, Colorado School of Mines — Far-field transmission spectra were obtained for structures consisting of subwavelength linear apertures flanked on one or both sides by periodic grating arrays in Au films. In each set of structures, the distance from the grating arrays to the aperture was incrementally varied. Transmission spectra clearly showed enhancement and suppression relative to an isolated aperture. A systematic shift in these extremes was observed with varying cavity width while holding other structural parameters constant. Distinct bands of enhancement and suppression arise from this analysis, consistent with a predictive analytical model. Our conclusions allow for precise control over enhancement-suppression at specific wavelengths in future structures.

\footnote{1}This material is based on work supported by the National Science Foundation under Grant No. DMI-0522281

12:39PM V44.00008 Lensless mapping and optical trapping. Christopher Dufort, Bogdan Dragnea, Chemistry Dept., Indiana University - Bloomington — Force mapping of optical gradients associated with electromagnetic fields above subwavelength apertures in a gold thin film has been studied using scanning probe techniques. Vertical cross-sections of this resulting field demonstrate that, in certain conditions, the light emerges in the form of a tightly focused beam even when the incident beam is only weakly focused. Quantification of the near-field in the vicinity of these apertures has shown it is possible to define a free particle resulting in an optical trapping effect. Applications involving lensless focusing below the diffraction limit and comparisons with traditional optical tweezing are discussed.

12:51PM V44.00009 Effective Non-Localities of Nano-Layered Meta-Materials, Justin Else, Viktor Podolskiy, Oregon State University, Ildar Salakhutdinov, Ivan Avrutsky, Wayne State University — Multi-layered nano-composites have been suggested for negative index of refraction systems, photonic funnels, super- and hyper-lenses, as well as other nanophotonic structures. We analyze the electromagnetic modes in such systems and show that they are not described by conventional effective-medium theories. We demonstrate the response of a majority of realistic layered structures is strongly affected by effective non-localities. We develop the analytical description of the relevant phenomena and confirm our results with rigorous numerical solutions of the Maxwell equations. Finally, we demonstrate that multi-layered plasmonic nanostructures support high-index volume modes confined to deep subwavelength areas by using the formalism we have developed.

1:03PM V44.00010 Fluorescence enhancement from silver nanostructures.\footnote{1}, Shyhaui Guo, Hunchih Kan, Ray Phaneuf, Univ. of Maryland, College Park — We report on experimental investigations of the fluorescence enhancement by nanotextured silver structures and its dependence on the incident light polarization and on the lateral periodicity. We find strong enhancement for TM mode polarization at smaller periods for thin spacer layers. Thicker spacer layers instead produce strong TE mode enhancement at small spacings.

\footnote{1}This work is supported by the Laboratory for Physical Science and an IC Postdoctoral Research Fellowship

1:15PM V44.00011 Influence of Local Field and Particle Plasmon on Fluorescence Enhancement from Spherical Nano-silver Particles.\footnote{1}, Shu-Ju Tsai, Hunchih Kan, Shy-Hau Guo, De-Hao Tsai, Michael Zachariah, Ray Phaneuf, University of Maryland — We report on investigation of fluorescence enhancement from silver nano-particles with selected diameters ranging from 50 nm to 320 nm. We measure the fluorescent intensity for two fluorophores, Cy3 and Cy5, coated on silver nano-particles deposited on silicon substrate using excitation source of an Ar ion laser at 514 nm and a HeNe laser at 633 nm, respectively. We find that the optimum diameter shifts to a larger value for the larger wavelength fluorophore; this is consistent with the particle plasmon–resonance dependence on particle size. However, we find that while the fluorescence enhancement drops sharply for larger particle sizes the extinction coefficient doesn’t. To understand this inconsistency, we perform numerical calculation with the discrete dipole approximation (DDA) method to calculate the extinction coefficient and the electric field strength near a single Ag particle on Si substrate. In comparison with measurement, the local field strength near the particle shows a size dependence in qualitative agreement with the fluorescence, the extinction coefficient does not.

\footnote{1}This work is supported by the Laboratory for physical Science and an IC Postdoctoral Research Fellowship

1:27PM V44.00012 Ultra-long range surface plasmon modes.\footnote{1}, Charles G. Durfee, Reuben T. Collins, Thomas E. Furtak, Colorado School of Mines, Russell E. Hollingsworth, ITN Energy Systems — It is well known that the propagation length of surface plasmon waves can be extended by exciting the appropriate mode of an isolated noble metal layer. The losses, however, increase substantially as the refractive index of the surrounding medium increases. Using a transfer matrix calculation, we have discovered that a thin, low-index dielectric adjacent to the metal layer can increase the intrinsic propagation length arbitrarily as the bound mode approaches cutoff. This geometry can be implemented in structures that combine metal-oxide-semiconductor (MOS) fabrication with plasmonic waveguides.

\footnote{1}This work was supported by the Air Force Office of Scientific Research.
the ratio between the Fermi and gauge field velocities. A common single disorder threshold is found to drive interchain and in-chain resistivities into a low temperature regime, consistent with many previous theoretical proposals, coherent hopping between chains appears to remain a relevant perturbation within the disordered system.

The emergence of an antiferromagnetic order can be described as the dynamical generation of mass due to the phenomenon of spontaneous chiral symmetry breaking. The theory predicts the Fermi surface of the pseudogap state \( \rho_s(T) \) and \( \rho_d(T) \) to be exponentially activated. In \( \rho_s(T) \), the two multiplets, the Zhang-Rice singlet and the Hund's coupling triplet, become nearly degenerate, and thus the \( \rho_s(T) \) remains a function of disorder content, introduced either through atomic-site substitution or electron irradiation. A common single disorder threshold is found to drive interchain and in-chain resistivities into a low temperature regime.

Pseudogap State of High-T\(_c\)cuprates. HIROSHI KAMIMURA, Tokyo University of Science — Undoped cuprates are Jahn-Teller (JT) Materials \cite{1,2} and Mott AF insulators \cite{2}. When holes are doped, the octahedrons or pyramids elongated by the JT effect shrink. We call such distortion against the JT effect "anti-Jahn-Teller effect" \cite{3}. By the interplay of the anti-Jahn-Teller effect and Mott physics, the two multiplets, the Zhang-Rice singlet and the Hund’s coupling triplet, become nearly degenerate, and thus the \( \rho_s(T) \) remains a function of disorder content, introduced either through atomic-site substitution or electron irradiation. A common single disorder threshold is found to drive interchain and in-chain resistivities into a low temperature regime.

Using analytic and FDTD calculations we present some of the consequences of CSP's on EOT as well as experimental confirmation of such effects. We find that EOT, even with cylindrical apertures, is aided by the increase in cutoff wavelength due to CSP’s, which is a consequence of the mode structure of individual apertures. CSP effects also explain most of the long-wavelength features of transmission spectra measured for CR apertures. We also show that CSP’s can be “spoofed” at low frequencies by coaxial apertures in metamaterials consisting of a (macroscopic) periodic dielectric structure embedded in a perfect conductor.

3:06PM W8.00002 Effects of Inhomogeneous Magnetic Correlations on the Penetration Depth in d-Wave Superconductors\(^1\), WILLIAM ATKINSON, Trent University — The influence of static magnetic correlations on the temperature-dependent superfluid density \( \rho_s(T) \) is calculated for d-wave superconductors. In self-consistent calculations, itinerant holes form incommensurate spin density waves (SDW) which coexist with superconductivity. In the clean limit, the density of states is gapped, and \( \rho_s(T \ll T_c) \) is exponentially activated. In inhomogeneously-doped cases, the SDW are disordered and both the density of states and \( \rho_s(T \ll T_c) \) exhibit an anomalous behavior.

3:30PM W8.00004 Critical Number of Fermions in Anisotropic QED; Application to the Pseudogap State of High-T\(_c\), Cuprates\(^1\), ANDRES CONCHA, VALENTIN STANEV, ZLATKO TESANOVIC, Johns Hopkins University — The low-energy physics of d-wave superconductors is marked by the presence of four nodal points where the gap function vanishes. This nodal structure can be used as the basis of an effective theory for fermionic quasiparticles, which turns out to be an incarnation of a two-dimensional quantum electrodynamics (QED\(_2\)), where the gauge field encodes quantum fluctuations in the phase of the gap function. The theory predicts the Fermi surface of the pseudogap state which is confined to the four nodal points and contains an intrinsic anisotropy reflecting the difference between the gap and Fermi velocities. In this context, the emergence of an antiferromagnetic order can be described as the dynamical generation of mass due to the phenomenon of spontaneous chiral symmetry breaking. Mass generation occurs when the number of fermionic species in the theory is less than some critical number \( N_c \), the actual value of which is still much debated. Based on simple physical arguments we find that \( N_c \) does depend on anisotropy and, more surprisingly, different regimes emerge depending on the ratio between the Fermi and gauge field velocities.

\(^1\)Supported by NSERC of Canada

\(^{2}\)Supported in part by NSF Grant DMR-0531159.
3:42PM W8.00005 Properties of the “quasi-particles” at a nodal nematic quantum critical point. EUN-AH KIM, PAUL ORETO, STEVE. KIVELSON, Stanford University, EDUARDO FRADKIN, UIUC — We study the properties of a d-wave superconductor in the vicinity of a quantum critical transition to a nematic (or d + s superconducting) phase. Most interactions have little effect on nodal quasiparticles, due to the limited phase space available for scattering. The few critical modes that do couple effectively (such as the phase fluctuations treated in the context of QED3) produce a renormalized (fixed point) dispersion that is isotropic (pseudo-Lorentz invariant). This contrasts with the extreme anisotropy found in ARPES experiments on cuprate superconductors, which is often considerably larger even than anticipated from mean-field considerations based on the magnitude of \( \Delta_0 / E_F \). We find quantum fluctuations near a nodal nematic quantum critical point strongly enhance the dispersion anisotropy, and are efficient inelastic scatterers. The quantum field theory which describes the nodal nematic critical point is non-Lorentz invariant and the nodal quasiparticles display clear non-Fermi liquid behavior. The fermion spectral function displays nontrivial structure, which can be compared with those measured by ARPES in cuprate superconductors.

3:54PM W8.00006 Excitons in QED\(_3\) and spin response in a phase-fluctuating d-wave superconductor\(^1\), BABAK SERADJEH\(^2\), University of British Columbia, IGOR HERBUT, Simon Fraser University — We study the particle-hole exciton mode in the QED\(_3\) theory of a phase-fluctuating d-wave superconductor in ladder approximation. We derive a Schrödinger-like equation for the exciton bound state and determine the conditions for its existence. We find the dispersion of this mode below the particle-hole continuum and compare our results with the resonance observed in neutron scattering measurements in cuprates. See http://www.physics.ubc.ca/~babak/march07/ for a list of references on this work.

3:06PM W8.00007 Effects of inhomogeneities and thermal fluctuations on the spectral function of a model d-wave superconductor\(^1\), DANIEL VALDEZ-BALDERAS, DAVID STROUD, Department of Physics, The Ohio State University — We compute the spectral function of a model for high-temperature superconductors, at both zero and finite temperatures \( T \). The model consists of a two-dimensional BCS Hamiltonian with d-wave symmetry, which has a spatially varying, thermally fluctuating, complex gap \( \Delta \). Thermal fluctuations are governed by a Ginzburg-Landau free energy functional. We assume that a fraction \( c_{ij} \) of the superconductor area has a large \( \Delta \) (\( J \)) regions, while the rest has a smaller \( \Delta \) (\( \alpha \) regions). \( \alpha \) and \( \beta \) regions are randomly distributed in space. We find that the inhomogeneous gap distribution of \( \Delta \) affects the spectral function primarily near \( k = (\pi, 0) \). For \( c_{ij} \approx 0.5 \), a split band appears if the difference between the gap magnitudes in the \( \alpha \) and \( \beta \) regions is sufficiently large; otherwise, the band is only broadened. Thermal fluctuations also affect the spectral function most strongly near \( k = (\pi, 0) \), where the peaks that are sharp and high at zero temperature become reduced, widened, and shifted toward smaller energies as \( T \) increases through the Kosterlitz-Thouless transition temperature.

4:06PM W8.00008 Enhanced superconductivity due to inhomogeneous bond order in a doped Mott insulator, JUN LIU, JOERG SCHMALIAN, Iowa State University, NANDINI TRIVEDI, Ohio State University — At half filling, the ground state of SrCu2(BO3)\(_2\), a half filled Mott insulator on the Shastry-Sutherland lattice, is exactly described by a valence bond wave function. Using a resonating valence bond wavefunction for the doped system, that includes the correct limit at half-filling, we find that the doped quantum magnet shows long ranged superconducting order. The superconductivity is boosted by the spontaneous emergence of a checker board pattern of the pairing strength on the bonds. We further find a strong asymmetry between hole and electron doping.

4:30PM W8.00009 Mott transition in Kagomé lattice Hubbard model, TAKUMA OHASHI, Condensed Matter Theory Laboratory, RIKEN, NÓRIO KAWAKAMI, Department of Physics, Kyoto University, HIROKAZU TSUNETSUGU, Institute for Solid State Physics, University of Tokyo — We investigate the Mott transition in the Kagomé lattice Hubbard model using the cellular dynamical mean field theory. The calculation of the double occupancy, the density of states, the static and dynamical spin correlation functions demonstrates that the system undergoes the first-order Mott transition at the Hubbard interaction \( U/W \approx 1.4 \) (\( W \): bandwidth). In the metallic phase close to the Mott transition, we find the strong renormalization of three distinct bands, giving rise to the formation of heavy quasiparticles with strong frustrated interactions. It is elucidated that the quasiparticle states exhibit anomalous behavior in the temperature-dependent spin correlation functions. We also find a dramatic change of the dominant spin fluctuations around the Mott transition. The spin fluctuations in the insulating phase favor down to the lowest temperature a spatial spin configuration in which the spin susceptibility representation of the particle-particle irreducible vertex. We find that with an effective temperature dependent coupling\(^2\), responsible for d-wave pairing in the doped two-dimensional Hubbard model with an on-site Coulomb interaction \( U \). Motivated by recent experiments suggesting sizeable lattice effects in the cuprates raise the issue of the role of electron-phonon (e-ph) interaction in strongly correlated systems. By means of Dynamical Mean-Field Theory, we show that, in the Hubbard-Holstein model, antiferromagnetic (AF) correlations strongly enhance the effects of the e-ph coupling with respect to the paramagnetic phase, even though the net effect of the Coulomb interaction is a moderate suppression of the e-ph interaction. Doping weakens the AF correlations and reduces the effects of the e-ph, leading to a scenario in which the tendency to polaron formation is weakened by doping, in agreement with the experimental results\(^3\).

1Work supported through National Science Foundation grant DMR04-13395 and by the Ohio Supercomputer Center.

4:42PM W8.00010 Spin susceptibility representation of the pairing interaction for the two-dimensional Hubbard model\(^1\), THOMAS MAIER, Oak Ridge National Laboratory, MARK JARRELL, University of Cincinnati, DOUGLAS SCALAPINO, University of California, Santa Barbara — We will discuss recent dynamic cluster quantum Monte Carlo studies of the effective pairing interaction responsible for d-wave pairing in the doped two-dimensional Hubbard model with an on-site Coulomb interaction \( U \) equal to the bandwidth. Motivated by earlier studies that show that the dominant contribution to the pairing interaction comes from the spin = 1 channel, we study a simple spin susceptibility representation of the particle-particle irreducible vertex. We find that with an effective temperature dependent coupling \( U(T) \) and the numerically calculated spin susceptibility \( \chi(K - K') \), the d-wave pairing interaction is well approximated by \( U(T) \chi(K - K') \).

1This work was supported by the Center for Nanoparticle Materials Sciences at Oak Ridge National Laboratory and by NSF DMR-0312680.

4:54PM W8.00011 Electron-Phonon Interaction and Antiferromagnetic Correlations, GIORGIO SANGIOVANNI, OLLE GUNNARSSON, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany, ERIK KOCH, Institut für Festkörperforschung, Jülich, Germany, CLAUDIO CASTELLANI, MASSIMO CAPONE, Department of Physics, University of Rome “La Sapienza”, Rome, Italy — Recent experiments suggesting sizeable lattice effects in the cuprates raise the issue of the role of electron-phonon (e-ph) interaction in strongly correlated systems. By means of Dynamical Mean-Field Theory, we show that, in the Hubbard-Holstein model, antiferromagnetic (AF) correlations strongly enhance the effects of the e-ph coupling with respect to the paramagnetic phase, even though the net effect of the Coulomb interaction is a moderate suppression of the e-ph interaction. Doping weakens the AF correlations and reduces the effects of the e-ph, leading to a scenario in which the tendency to polaron formation is weakened by doping, in agreement with the experimental results\(^1\).

mass is temperature dependent and increases from 1.5 at room temperature to 2.5 just above $T_c$.

This is the same frequency at which the optical conductivity shows a clear loss of spectral weight in the superconducting state. The low frequency effective $\omega^2$ phenomenologically, however, gives a very good description of the change in optical spectral weight at $T_c$.

We demonstrate that a new tool, a model independent numerical Eliashberg inversion of the optical self-energy, based on maximum entropy considerations can be used to extract the magnetic excitation spectra of high-transition-temperature superconductors. In Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ we explicitly show that the magnetic mode that dominates the self-energy at low temperatures directly evolves out of a smooth transfer of spectral weight to the mode from the continuum just above it. This redistribution starts already at 200 K in optimally doped materials but is much weaker in overdoped samples. This provides evidence for the magnetic origin of the superconductivity and presents a challenge to theories of the spin susceptibility and to neutron scattering experiments in high-transition temperature superconductors.

We investigated the ab-plane infrared and visible spectra of a HgBa$_2$CuO$_4$ single crystal close to optimal doping ($T_c=97$ K). Optical spectra have been obtained with a high temperature resolution allowing us to track small changes in the integrated spectral weight. We find that the low frequency spectral weight shows an extra increase when the system enters the superconducting state, indicating that the kinetic energy of the charge carriers decreases in the superconducting state. This is consistent with our earlier observations on other optimally doped cuprates. We find that changes of both signs can occur within a conventional BCS framework. Using a band structure determined for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, we find that a straightforward BCS calculation of the optical spectral weight cannot account for the experimental observations. Including a scattering rate collapse phenomenologically, however, gives a very good description of the change in optical spectral weight at $T_c$ as a function of doping.

We use a new technique to directly extract an estimate of the quasiparticle self-energy from the optical conductivity which can be easily related to both theory and angle-resolved photoemission spectroscopy (ARPES) experiments. In the high $T_c$ cuprate Bi-2212 we find evidence for a new high energy scale at 900 meV in addition to the two previously well known ones at roughly 50 and 400 meV. The intermediate scale at 400 meV has been recently seen in ARPES as a large kink which optics finds to be weaker and shifted. In YBCO, the three energy scales are shifted to lower energy relative to Bi-2212 and we observe the emergence of a possible fourth high energy feature at 600 meV.

High energy scales in electronic self-energy imaged by optical conductivity

We use a new technique to directly extract an estimate of the quasiparticle self-energy from the optical conductivity which can be easily related to both theory and angle-resolved photoemission spectroscopy (ARPES) experiments. In the high $T_c$ cuprate Bi-2212 we find evidence for a new high energy scale at 900 meV in addition to the two previously well known ones at roughly 50 and 400 meV. The intermediate scale at 400 meV has been recently seen in ARPES as a large kink which optics finds to be weaker and shifted. In YBCO, the three energy scales are shifted to lower energy relative to Bi-2212 and we observe the emergence of a possible fourth high energy feature at 600 meV.

High energy kinks in the Cuprates

5:06PM W8.00012 High Energy Kinks in the Cuprates, R.S. MARKIEWICZ, S. SAHRAKORPI, A. BANSIL, Northeastern University — Tunneling studies in conventional superconductors are well known to reveal details of the electron-phonon interaction responsible for pairing. Similar features—low energy kinks in the 40-70 meV range—have also been observed in the cuprates, but their origin and possible role in pairing have been hotly debated. Recently, even higher energy kinks above 200 meV have been reported in the ARPES spectra of several cuprates. In this connection we discuss the roles of electron-plasmon as well as electron-magnon effects and show that collective modes in the charge and spin channels in the cuprates yield band renormalizations at low energies and anomalous features in band dispersion at higher energies, which are in substantial accord with experimental results.

5:18PM W8.00013 ABSTRACT HAS BEEN MOVED TO P8.00003 –

Thursday, March 8, 2007 2:30PM - 5:18PM –

Session W9 DMP: Superconductivity: Optical and Raman Spectroscopy Colorado Convention Center Korbel 1D

2:30PM W9.00001 Evolution of the Spin Susceptibility of High-$T_c$ Superconductors, THOMAS TIMUSK, JUNGSEEK HWANG, McMaster University, EWALD SCHACHINGER, Graz University of Technology, JULES CARBOTTE, McMaster University — We present optical spectra and specific heat measurements of the behavior of the electron doped Pr$_1$Ce$_{18}$Sr$_2$O$_{44}$ and hole doped cuprates is suppressed to about 25% of value predicted by band structure.

Supported by NSF # DMR-0030112

2:42PM W9.00002 Intraband Optical Spectral Weight in the presence of a Van Hove singularity: application to Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, FRANK MARSIGLIO, University of Alberta, FABRIZIO CARBONE, ALEXEY KUZMENKO, DIRK VAN DER MAREL, Universite de Geneve — While the Kubo sum rule is often applied to the entire optical spectral weight to learn about the bare plasma frequency, the so-called “Kubo single band sum rule” is used to determine the optical spectral weight corresponding to intraband transitions in the valence band. We use a tight binding band with further than nearest neighbour hopping to explore the range of superconductivity-induced changes that are possible. We find that changes of both signs can occur within a conventional BCS framework. Using a band structure determined for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, we find that a straightforward BCS calculation of the optical spectral weight cannot account for the experimental observations. Including a scattering rate collapse phenomenologically, however, gives a very good description of the change in optical spectral weight at $T_c$ as a function of doping.

Supported by NSERC, ICORE, CIAR (Canada) and MaNeP (Switzerland)

2:54PM W9.00003 Hall conductivity spectral weight in electron and hole doped cuprates, H. D. CREW, Physics Department, University of Maryland, College Park, MD — The optical conductivity quasiparticle spectral weight in optimally electron and hole doped cuprates is suppressed to about 25% of value predicted by band structure. This suppression is due to Mott-Hubbard correlations caused by strong Coulomb interactions. These correlations inter the longitudinal conductivity and the Hall conductivity differently. We have investigated the Fermi-liquid like behavior of the electron doped Pr$_1$Ce$_{18}$Sr$_2$O$_{44}$ slightly overdoped and optimally hole doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ using a spectral weight analysis of the Hall conductivity. In both materials the Hall conductivity spectral weight was found to be suppressed to about 10% of the band value. This more substantial suppression of the Hall spectral weight addresses fundamental questions concerning the effects of Mott and antiferromagnetic correlations on the transport properties of strongly correlated materials.

Supported by NSF # DMR-0030112

3:06PM W9.00004 High energy scales in electronic self-energy imaged by optical conductivity, E. J. NICOL, University of Guelph, J. HWANG, T. TIMUSK, McMaster University, A. KNIGAVKO, Brock University, J. P. CARBOTTE, McMaster University — We use a new technique to directly extract an estimate of the quasiparticle self-energy from the optical conductivity which can be easily related to both theory and angle-resolved photoemission spectroscopy (ARPES) experiments. In the high $T_c$ cuprate Bi-2212 we find evidence for a new high energy scale at 900 meV in addition to the two previously well known ones at roughly 50 and 400 meV. The intermediate scale at 400 meV has been recently seen in ARPES as a large kink which optics finds to be weaker and shifted. In YBCO, the three energy scales are shifted to lower energy relative to Bi-2212 and we observe the emergence of a possible fourth high energy feature at 600 meV.

3:18PM W9.00005 Optical and thermodynamic properties of Hg-1201, E. VAN HEUMEN, R. LORTZ, F. CARBONE, A.B. KUZMENKO, D. VAN DER MAREL, Universite de Geneve, X. ZHAO, G. YU, Y. CHO, N. BARIK, M. GREVEN, Stanford university, C.C. HOMES, Brookhaven National Laboratory, S.V. DORDEVIC, Akron University — We present optical spectra and specific heat measurements of the optimally doped, single layer cuprate superconductor HgBa$_2$Cu$_2$O$_4$ ($T_c=97$ K). Optical spectra have been obtained with a high temperature resolution allowing us to track small changes in the integrated spectral weight. We find that the low frequency spectral weight shows an extra increase when the system enters the superconducting state, indicating that the kinetic energy of the charge carriers decreases in the superconducting state. This is consistent with our earlier observations on other optimally doped cuprates.

From specific heat measurements on the same sample we estimate the change of the kinetic energy of the system, which is given by $\Delta U$ in MeV per copper and $\Delta W=0.1$ MeV per copper for the kinetic energy.

3:30PM W9.00006 Optical conductivity of single plane cuprate superconductor HgBa$_2$CuO$_4$, R.P.S.M. LOBO, N. BONTEMPS, CNRS-ESPCI, Paris, France, J. HWANG, J. YANG, T. TIMUSK, McMaster University, Hamilton, Canada, D. COLSON, A. FORGET, DREAM/SPEC, CEA, Saclay, France — We investigated the ab-plane infrared and visible spectra of a HgBa$_2$CuO$_4$ single crystal close to optimal doping ($T_c=90$ K) from 100 to 40000 cm$^{-1}$. Data as a function of temperature (down to 30 K) was limited to frequencies below 10000 cm$^{-1}$. The low frequency scattering rate has a linear frequency dependence. Under 120 K a supplementary small drop below 1000 cm$^{-1}$ suggests the presence of a pseudogap. This is the same frequency at which the optical conductivity shows a clear loss of spectral weight in the superconducting state. The low frequency effective mass is temperature dependent and increases from 1.5 at room temperature to 2.5 just above $T_c$. We will compare our results to other single plane cuprates.

$\Delta U=0.1$ MeV per copper and $\Delta W=0.1$ MeV per copper for the kinetic energy.

Supported by NSERC, ICORE, CIAR (Canada) and MaNeP (Switzerland)
3:42PM W9.00007 Visible Pump-THz Probe Spectroscopy of the Undoped Cuprate Sr$_{2}$CuCl$_{4}$. JESSE PETERSEN, J. STEVEN DODGE, Simon Fraser University, RUIXING LIANG, University of British Columbia — We present experimental results on the mobility of photoexcited carriers in Sr$_{2}$CuCl$_{4}$ on an undoped cuprate. We use ultrashort laser pulses to excite photoexcitons in the antiferromagnetic insulating lattice. We then probe the low-frequency dynamical conductivity of this nonequilibrium state with time-domain terahertz spectroscopy. Our current measurements place an upper bound on the mobility that is consistent with Hall mobility measurements.[1]


3:54PM W9.00008 Small Magnetic Fields Arrest the Josephson Plasma Resonance in La$_{2+3x}$Sr$_{x}$CuO$_{4}$ for x=1/8. ALEXANDER SCHAFGANS, ANDREW LAFORGE, Department of Physics, University of California San Diego, SASA DORDEVIC, Department of Physics, The University of Akron, SEIKI KOMIYA, YOICHI ANDO, Central Research Institute of Electric Power Industry, Tokyo, Japan, DIMITRI BASOV, Department of Physics, University of California San Diego — We report on a study of the far infrared interlayer response in a La$_{2+3x}$Sr$_{x}$CuO$_{4}$ (La214) crystal at the x=1/8 doping. A magnetic field up to 8 Tesla, applied perpendicular to the CuO$_{2}$ planes, is found to completely suppress the Josephson plasma resonance (JPR) in sharp contrast to the mild suppression of the JPR if the field is applied along the planes. We suggest that this anomalous sensitivity of the JPR feature to modest fields for Hc-axis is due to the interaction of in-plane charge inhomogeneities with vortices that form in the CuO$_{2}$ planes.

4:06PM W9.00009 Order parameter of the paired hole states in Sr$_{14}$Cu$_{2}$O$_{11}$ studied by optics and UV-resonance Raman scattering. ANDRIVDO ROUSYDI, B. SCHULZ, R. RAUER, I. MAHNS, University of Hamburg, H. EISAKI, Nanoelectronics Research Institute, AIST, Y. FUJIMAKI, S. UCHIDA, University of Tokyo, P. ABBAMONTE, University of Illinois, M. RÜBHAUSEN, University of Hamburg — The order parameter of the paired hole states at hole Wigner crystal (HC) in the self-doped spin (S)1/2 two-leg ladders of Sr$_{14}$Cu$_{2}$O$_{11}$ (SCO) is studied with optics and UV-resonance Raman scattering. We observe a pair breaking excitation of the holes (2Δ$_{a}$,c) at 200 meV which can be attributed to the rungs of the ladders. The intensity of the 2Δ$_{a}$,c peak as function of temperature matches very well with the formation of HC at about 250 K ($T_{HC}$). The energy of 2Δ$_{a}$,c is temperature independent, even at its transition temperature indicating a remaining short range order with a strongly decreased volume fraction. The order parameter of the paired hole states develops in a non-mean-field fashion and 2Δ$_{a}$,c/k$_{B}T_{HC}$ is about 11, i.e. in the strong coupling limit. Our optics studies also show low- and high-spin transitions along the legs and rungs below 130 K. Our measurements confirm theoretical predictions of the existence of the paired hole states outlining the strong local pairing of the holes.

4:18PM W9.00010 Ultrafast Observation of the Coexistence of Antiferromagnetism and Superconductivity in the High-T$_{c}$ Superconductor Ti$_{2}$Ba$_{2}$Ca$_{2}$Cu$_{3}$O$_{y}$. ELBERT E.M. CHIA, JIAN-XIN ZHU, D. TALBAYEV, A.J. TAYLOR, R.D. AVERITT, Los Alamos National Laboratory, IN-SUN JO, KYU-HWAN OH, SUNG-IK LEE, Pohang University — In high-T$_{c}$ superconductors (HTSC), it is commonly believed that Cooper pairing occurs via antiferromagnetic spin fluctuations. These spin fluctuations can be shown to exist if the competing ground state to the superconducting (SC) state is antiferromagnetism (AFM). It reveals itself when, for example, the SC state is destroyed or suppressed using an externally applied magnetic field. Ultrafast spectroscopy has been widely used in probing the relaxation dynamics of photoexcited quasiparticles in correlated electron systems, and in particular, cuprate HTSCs. However, no such measurements have been taken for the regime where AFM and SC might possibly coexist. We report the first ultrafast relaxation measurements in such a coexistence phase in the HTSC Ti$_{2}$Ba$_{2}$Ca$_{2}$Cu$_{3}$O$_{y}$. Without applying any external magnetic field, we see a (TDCS) negative change in the relaxation dynamics below ~40 K, which is suggestive of an (entry) into the AFM-SC coexistence phase. To quantitatively explain our data, we combined a coupled model describing the time-evolution of quasiparticles and high-frequency photons in the presence of a gap in the density of states, and a mean field model that gives rise to a decrease in the SC gap as one enters the coexistence state.

4:30PM W9.00011 Electron-phonon coupling in SrTi$_{1−x}$Nb$_{x}$O$_{3}$. D. VAN MECHELEN, P. ARMITAGE, Universite de Geneve, C. GRIMALDI, EPFL, A. KUZMENKO, J. TEYSSIER, D. VAN DER MareL, Universite de Geneve — One of the major questions in the physics of high temperature is, to what extent electron-phonon coupling is important for the transport anomalies and for the superconductivity itself. One of the difficulties in addressing this issue for the cuprates, is the complexity of these materials, which are doped Mott-insulators, anti-ferromagnetic, striped, etcetera. In order to separate out the electron-phonon coupling we have studied the perovskite SrTi$_{1−x}$Nb$_{x}$O$_{3}$ with 0.0002 < x < 0.02. The lowest uncoupled bands of pristine SrTiO$_{3}$ are Ti 3d bands of t$_{2g}$ character, which become occupied with electrons upon substituting Nb for Ti. Here we report THz, infrared and optical spectra, DC resistivity and Hall effect. The infrared spectra at 7 K reveal a very narrow (less than 2 meV) Drude peak, the spectral weight of which reveals a strong electron-phonon coupling. The energy of the 2h$_{c}$,h peak as function of temperature matches very well with the formation of HC at about 250 K ($T_{HC}$). The energy of 2h$_{c}$,h is temperature independent, even at its transition temperature indicating a remaining short range order with a strongly decreased volume fraction. The order parameter of the paired hole states develops in a non-mean-field fashion and 2h$_{c}$,h/k$_{B}T_{HC}$ is about 11, i.e. in the strong coupling limit. Our optics studies also show low- and high-spin transitions along the legs and rungs below 130 K. Our measurements confirm theoretical predictions of the existence of the paired hole states outlining the strong local pairing of the holes.

[1] This work was supported by the Swiss National Science Foundation through the National Center of Competence in Research “Materials with Novel Electronic Properties-MaNEP”.

4:42PM W9.00012 First demonstration of a superconducting detector cooled by solid-state refrigerators. N.A. MILLER[1,2], J.A. BEALL[1], D.J. BENFORD[1], T.C. CHEN[1], J.A. CHERVENAK[1], W.D. DUNCAN[1], F. FINKBEINER[1], G.C. HILTON[1], K.D. IRWIN[1], S.H. MOSELEY[1], G.C. O’NEIL[1,2], D.R. SCHMIDT[1], L.R. VALE[1], R.F. SILVERBERG[1], J.N. ULLOM[1] — We have successfully cooled a Transmission Electron Microscope (TEM) stage to 8 K using a solid-state refrigerator. This is a new mechanism for achieving ultra-low temperatures in the TEM which has potential applications for materials science research. The cooling mechanism is the preferential tunneling of the highest energy (hottest) electrons through the biased NIS junctions. We describe the cooling performance, temperature noise, and energy resolution of the NIS-cooled TES. In particular, we show that the NIS refrigerators introduce no detectable noise in the TES operation. NIS refrigerators can cool from temperatures near 0.3 K to below 0.1 K. Combining a pumped He system with NIS refrigerators provides a compact, lightweight alternative to adiabatic demagnetization refrigerators and dilution refrigerators. Bath temperatures near 0.1 K are desirable for state-of-the-art sensors for astronomy and materials analysis, as well as for a wide range of basic science applications. The National Institute of Standards and Technology (NIST) — Boulder[2]University of Colorado at Boulder[2]NASA/Goddard Space Flight Center[2]Global Science and Technology[2]SSAI.

4:54PM W9.00013 Fast, Single-photon Detection with Superconducting Niobium Nanowires. ANTHONY ANNUNZIATA, Yale University, AVIAD FRYDMAN, Bar Ilan University, MICHAEL ROOKS, IBM T. J. Watson Research Center, DANIEL PROBER, Yale University — We present recent measurements of the quantum efficiency, counting rate, and dark count rate for single-photon detectors based on superconducting niobium nanowires at 337 nm and 470 nm wavelengths for several detector geometries. From this data it is shown that the reset time (and therefore the single-photon counting rate) of these detectors is not dependent on the kinetic inductance of the niobium wire, as is the case for other detectors of this type made from niobium-nitride. The counting rate approaches 1 GHz even for very large area (100 µm$^{2}$) detectors. A phenomenological model of detection is presented that suggests the ability to resolve the number of photons absorbed during individual detection events. Preliminary data is shown that supports this assertion. These detectors have a variety of potential applications ranging from VLSI circuit diagnostics to quantum communication and single molecule spectroscopy. This work is supported by NSF and IBM research.
5:06PM W9.00014 Antenna-Coupled Superconducting Bolometers for Studying Dynamics with Terahertz Spectroscopy

Department of Physics and Astronomy, UC Riverside, R. KAWAKAMI, Department of Physics and Astronomy, UC Riverside, J. STEPHENS, D. AWSCHALOM, Center for Spintronics and Quantum Computation, UC Riverside — We report microwave and terahertz characterizations of antenna-coupled hot electron bolometers designed for laboratory-based terahertz spectroscopy. The active element is a superconducting niobium microbridge, and the incident signal is coupled to the microbridge by a planar double-dipole antenna. These devices combine sub-nanosecond response with high sensitivity and the ability to operate below saturation when viewing a room temperature background. The optimum small signal responsivity is $4.4 \times 10^4$ V/W, obtained at a bath temperature $T_b \approx 0.9T_c$. The corresponding saturation power is $7\text{ nW}$. The saturation power increases and the responsivity decreases as the bath temperature is lowered. The measured noise equivalent power is $2.0 \times 10^{-14}$ W/(Hz)$^{1/2}$, near the predicted thermal fluctuation limit. The unique combination of speed and sensitivity demonstrated by these detectors will enable new measurements of dynamic processes in the far-infrared on millisecond to nanosecond timescales.

1This work was supported by NSF-CHE and NSF-AST.

Thursday, March 8, 2007 2:30PM - 5:30PM –
Session W12 GMAG DMP FIAP: Focus Session: Spin Dependent Tunneling II
Colorado Convention Center Korbel 3C

2:30PM W12.00001 Spin polarization of electrons in 2D structures due to reflection from a barrier

V. T. T. ODORESCU, Department of Physics, Northern Illinois University, DeKalb, IL 60115, R. WINKLER, Department of Physics, Northern Illinois University, DeKalb, IL 60115 and Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439 — In two-dimensional semiconductor structures Rashba spin-orbit coupling can orient the electron’s spin in two opposite directions perpendicular to the direction of motion. We analyze here the possibility to change the spin polarization of an electron beam which is reflected from a barrier in the 2D plane. In general, an unpolarized incident beam gives rise to three reflected beams with different polarizations [1]. We give the orbital and spin parts of the current densities inside and outside of the interference zones. Also we estimate for an initially unpolarized (or partially polarized) electron beam the change of the degree of polarization due to multiple reflections between two parallel barriers in a ballistic regime using realistic material parameters. [1] A. O. Govorov et al., Phys. Rev. B 70, 245310 (2004)

1Research at Argonne was supported by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. Research at NIU was supported by the Department of Education.

2:42PM W12.00002 Spin-dependent properties of Fe/MgO/GaAs heterostructures

Y. LI, Y. CHYE, Y. CHANG, Department of Physics and Astronomy, UC Riverside, J. STEPHENS, D. AWSCHALOM, Center for Spintronics and Quantum Computation, UC Santa Barbara, R. KAWAKAMI, Department of Physics and Astronomy, UC Riverside — Developing efficient spin injectors and spin detectors is an important goal for semiconductor-based spintronics. Recently Jiang et al.’s work using CoFe/MgO tunnel spin injectors showed significantly enhanced spin injection efficiency into GaAs due to a spin filtering effect of the MgO layer [a]. Using molecular beam epitaxy (MBE) deposition, we have successfully grown atomically flat MgO films on GaAs(001) epilayers. Below 2 nm thickness, the MgO films are found to be single crystalline. The spin-dependent properties of a Fe/MgO/GaAs heterostructure are investigated by time-resolved Faraday rotation (TRFR) to measure ferromagnetic proximity polarization (FPP) across MgO [b]. It is seen that a very small amount of MgO (less than 0.5 nm thickness) enhances the FPP significantly. We are investigating the FPP dependence on MgO thickness by scanning the optical beams across an MgO wedge. A systematic study on MgO thickness dependence will be presented and the mechanism of indirect FPP across MgO will be discussed. Supported by NSF, ONR, and CNID. (a) X. Jiang, et al., Phys. Rev. Lett. 94, 056601 (2005). (b) R. J. Epstein, et al., Phys. Rev. B 65, 121202 (2002)

2:54PM W12.00003 Magnetic field dependence of a resonant tunneling diode based in the GaMnAs/AlGaAs material system.

EDWARD LIKOVICH, KASEY RUSSELL, WEI YI, VENKATESH NARAYANAMURTI, Harvard University, KHEH-CHIANG KU, NIITU SAMARTH, Penn State University, NARAYANAMURTI TEAM, SAMARTH TEAM — A resonant tunneling diode was fabricated with magnetic GaMnAs emitter and quantum well regions and a nonmagnetic p-GaAs collector. At 4K, below the Curie temperature for GaMnAs, negative differential resistance (NDR) associated with resonant tunneling of holes was observed. Both the magnitude of NDR as well as its associated bias were found to be dependent on magnetic field. If the device bias is held constant and the magnetic field is swept, our device exhibits either positive or negative differential resistance (NDR) associated with resonant tunneling of holes. The barrier height of the heterojunction follows a Brillouin function with $S=7/2$, demonstrating that the transport is dominated by the large, near the predicted thermal fluctuation limit. The unique combination of speed and sensitivity demonstrated by these detectors will enable new measurements of dynamic processes in the far-infrared on millisecond to nanosecond timescales.

1currently at Princeton University

3:06PM W12.00004 Electron Tunneling across EuS / InAs Heterojunctions


3:06PM W12.00004 Electron Tunneling across EuS / InAs Heterojunctions

EDWARD LIKOVICH, KASEY RUSSELL, WEI YI, VENKATESH NARAYANAMURTI, Harvard University, KHEH-CHIANG KU, NIITU SAMARTH, Penn State University, NARAYANAMURTI TEAM, SAMARTH TEAM — A resonant tunneling diode was fabricated with magnetic GaMnAs emitter and quantum well regions and a nonmagnetic p-GaAs collector. At 4K, below the Curie temperature for GaMnAs, negative differential resistance (NDR) associated with resonant tunneling of holes was observed. Both the magnitude of NDR as well as its associated bias were found to be dependent on magnetic field. If the device bias is held constant and the magnetic field is swept, our device exhibits either positive or negative tunneling magetoresistance (TMR) up to several tens of percent, depending on the device bias.

1Work supported by ONR award #MDA972-02-1-0002.

3:30PM W12.00005 Tunneling Properties of a Magnetic Tunneling Diode


3:48PM W12.00006 Tunneling Properties of a Magnetic Tunneling Diode


3:18PM W12.00005 Digital magneto resistance in magnetic MOBILEs1, CHRISTIAN ERTLER, JAROSLAV FABIAN, Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — Resonant tunneling structures comprising magnetic semiconductor layers are promising for realizing efficient spin filters and detectors [1]. Recently [2], we showed that a paramagnetic MOBILE (Monostable-Bistable Transition Logic Element), which consists of two serial connected resonant tunneling diodes (RTDs), the nonmagnetic load and the driver with a paramagnetic quantum well (QW), exhibits digital magneto resistance (DMR): a continuous change of the external magnetic field above a threshold value leads to a discrete jump of the output voltage from low to high. We have also proposed a nonvolatile ferromagnetic MOBILE, where the driver-RTD comprises a ferromagnetic magnetic tunneling barrier, and the QW. We show that DMR is realized by changing the relative orientation of the magnetizations above a threshold angle. In the low voltage regime the driver IV can be changed from ohmic to negative differential resistance behavior. Since conventional MOBILEs have been demonstrated to work up to 100 GHz the proposed device might be useful for performing very fast detections of magnetic signals. [1] I. Zutic, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004). [2] C. Ertler and J. Fabian, Appl. Phys. Lett. 89, 193507 (2006).

1Supported by the Deutsche Forschungsgesellschaft SFB 689.

3:30PM W12.00006 Reversing the sign of the spin-polarized current across a Fe/GaAs tunnel barrier at finite voltage bias S.A. CROOKER, Los Alamos National Laboratory, X. LOU, C. ADELMANN, E.S. GARLID, J. ZHANG, S.M. REDDY, S.D. FLEXNER, C.J. PALMSTROM, P.A. CROWELL, University of Minnesota — As a function of the voltage bias across a Fe/GaAs Schottky tunnel barrier, we measure the sign and magnitude of the electrically-injected spin polarization in the semiconductor, $P_{GaAs}$, using magneto-optical Kerr rotation at 10 K. Both images and Hanle depolarization curves reveal that the sign of $P_{GaAs}$ inverts when sweeping from small reverse bias (electrons flowing into GaAs) to small forward bias (electrons flowing into Fe), as expected from linear response. More strikingly, $P_{GaAs}$ inverts sign again at higher bias across the Fe/GaAs barrier. This crossover bias ($|V_{dc}| < 0.1$ V in the structures studied) is sample-dependent, and can occur under either forward- or reverse-bias conditions, depending on sample. These data concur with all-electrical measurements of $P_{GaAs}$ in lateral spin transport devices having a source, drain, and a third 'non-local' detection electrode. Models to describe these data will be discussed. We further show that, when Fe/GaAs tunnel barriers are employed as electrical spin detectors, both the sign and magnitude of the detection sensitivity can be tuned with applied bias on the detector. This work is supported by the Los Alamos LDRD and NSF MRSEC programs, and ONR.

3:42PM W12.00007 Spin extraction theory and its spintronics applications1, HANAN DERY, LU J. SHAM, Department of Physics, University of California at San Diego — Extraction of electrons from a semiconductor to a ferromagnet as well as the case of injection in the reverse direction may be formulated as a scattering theory. However, the presence of bound states at the interface arising out of an inhomogeneous doping on the semiconductor side must be taken into account in the scattering theory. Inclusion of the interface states yields an explanation of a recent result of spin imaging measurement which contradicts the current understanding of spin extraction (S. A. Crooker et al., Science 309, 2191 (2005)). A particular consequence of our theory is a proposed electrically controlled spin-switch in which a non-magnetic back-gate monitors the spin polarization in a semiconductor. The switch also utilizes a ferromagnet field to either switch the spin species depending on the gate bias. Based on these ideas (and if time allows), we will present a semiconductor spintronic prototype of a reprogrammable, universal logic gate which does not require magnetic fields throughout its operation. (See also, cond-mat/0609045)

1This work is supported by NSF DMR-0325599.

3:54PM W12.00008 Spin-dependent tunneling properties in GaMnAs-based magnetic tunnel transistors YOSUKE MIZUNO, Dept. of Electronic Eng., The Univ. of Tokyo, SHINOBU OHYA, Dept. of Electronic Eng., The Univ. of Tokyo; PRESTO JST, PHAM NAM HAI, Dept. of Electronic Eng., The Univ. of Tokyo, MASAAKI TANAKA, Dept. of Electronic Eng., The Univ. of Tokyo; SORST JST — III-V-based ferromagnetic-semiconductor heterostructures comprising GaMnAs are hopeful candidates for future spintronic devices. Thus far, only two-terminal devices have mainly been studied. Meanwhile, GaMnAs-based ‘three-terminal’ magnetic tunnel transistors (MTTs) have a potential to add novel functions to integrated circuits. We prepared MTT structures comprised of GaMnAs (30 nm)/AlAs (2 nm)/GaMnAs (30 nm)/GaAs:Be (30 nm)/Si(1011) cm$^{-3}$ on p-GaAs(001) substrates using molecular-beam epitaxy (MBE). The $V_{EG}$ dependence of $I_{C}$, $I_{E}$, and $I_{B}$ shows that the current transfer ratio $\alpha (=I_{C}/I_{E})$ is 0.8-0.95; this is much higher than 0.30, the maximum value reported in metal-based MTTs. The current gain $\beta (=I_{E}/I_{B})$ is of the order of 10, which means that GaMnAs-based MTTs have current amplifiability. The $I_{CG}$ dependence of the tunneling magnetoresistance (TMR) ratio differed significantly from that observed in single-barrier magnetic tunnel junctions (MTJs). This work was partly supported by PRESTO / SORST of JST, Grant-in-Aids for Scientific Research, IT-R2002 of MEXT, and Kurata-Memorial Hitachi Sci. & Tech. Foundation.

4:06PM W12.00009 Resonant tunneling effect and tunneling magnetoresistance in ferromagnetic-semiconductor quantum heterostructures, SHINOBU OHYA, Dept. of Electronic Eng., The Univ. of Tokyo; PRESTO JST, PHAM NAM HAI, YOSUKE MIZUNO, Dept. of Electronic Eng., The Univ. of Tokyo, MASAAKI TANAKA, Dept. of Electronic Eng., The Univ. of Tokyo; SORST JST — Ferromagnetic-semiconductor quantum heterostructures are expected to realize novel functions by combining the resonant tunneling effect and the tunneling magnetoresistance (TMR). However, there are no reports on the clear observation of the resonant tunneling effect and TMR associated with it in these structures. We fabricated the GaMnAs quantum-well (QW) double-barrier heterostructures composed of GaMnAs(20 nm)/AlGaAs(4 nm)/GaMnAs(3/9.8-20 nm)/AlGaAs(4 nm)/GaAs:Be on p-GaAs(001) substrates using molecular-beam epitaxy (MBE). The $dV/dI$-V characteristics and bias dependence of TMR measured at 2.6 K clearly show oscillatory behaviors in the negative bias region where holes are injected from the GaAs:Be layer to the GaMnAs QW. With increasing d, the peaks of these oscillations shift to smaller voltages and the period becomes short, which indicates that they are induced by the resonant tunneling effect. This work was partly supported by PRESTO/SORST of JST, Grant-in-Aids for Scientific Research, IT Program of RR2002 of MEXT, and Kurata-Memorial Hitachi Science & Technology Foundation.

4:18PM W12.00010 Exchange Splitting and 100% Spin Polarization in Monolayer level EuO Films1, TIFFANY SANTOS, JAGADEESH MOODERA, Francis Bitter Magnet Lab, MIT, EZANA NEGUSSE, YVES IDZERDA, Montana State University — The exchange splitting of the conduction band in an ultrathin film of ferromagnetic EuO just 2.5 nm thick has been determined for the first time using tunneling techniques. In a Al/EuO/Y tunnel junction, a huge drop in junction resistance versus temperature was observed below the EuO Tc=69K, resulting from an exchange splitting of 0.3 eV, which corresponds to a spin filter efficiency of 98% ! Furthermore, substantial tunnel magnetoresistance (~ 280%) has been observed in Cu/EuO/Gd quasi-magnetic tunnel junctions. From these observations, it appears that EuO is approaching its theoretical spin polarization P of 100%. Whereas previously, a value of only 30% was obtained using the Meservey-Tedrow technique of directly measuring P. This drastic improvement occurred after examining the chemical and magnetic properties of EuO at the monolayer level and its interfacial properties with metals, using SQUID magnetometry, XAS, XMCD and XRS. With the right combination of interface materials and deposition parameters, one can have a 1nm EuO film with a high moment of >7 $\mu_B$. With this high spin filter efficiency and its compatibility with Si, the EuO spin filter shows promise for injecting highly-polarized spins into Si-based semiconductors.

1Supported by NSF and the KIST-MIT joint program.
4:30PM W12.00011 Room Temperature Tunneling Characteristics through SDT Nanoscaled Lines into n-Doped Si. YU ZHANG, NAM H. KIM, JIAN-QING WANG, SUNY-Binghamton, JIM DAUGHTON, NVE Corporation — Nanoscaled spin-dependent tunneling (SDT) lines were patterned on n-doped Si layer and studied for tunneling characteristics from ferromagnetic nano-lines through an AlOx insulating barrier into the semiconductor. The functional magnetic layering was deposited on doped Si with phosphorus (n-type) having resistivity of 0.006-0.02 Ohm-cm. The configuration of the SDT film is 1.5 nm AlOx / 4 nm NiFeCo / 1 nm FeCo / 15 nm Cu / 15 nm CrSi / 10 nm Si3N4 as spin injection contact. The patterned lines with width and separation of 100 nm were produced using e-beam lithography. The tunneling characteristics versus temperature (80 to 300 K) were measured by wire bonding and with assistance of ohmic contacts of heavily doped regions. The tunneling studied through the barrier between layered-magnetic metals and semiconductor clearly showed the electronic transport as ballistic tunneling, showing weakly dependence on the temperature. This is qualitatively different similarly scaled-up SDT line-structures with 2 micron gap distance. In the later configuration, the electronic transport was observed to be mainly thermal emission dominant process at elevated temperatures, with characteristic activation energy in agreement with the impurity level.

4:42PM W12.00012 Measuring Spin Dependent Hot Electron Transport in Fe/Si(001) Schottky Diodes1. ANDREW STOLLENWERK, University at Albany, MICHAEL KRAUSE, Thomson, JOHN GARRAMONE, EVAN SPADAFORA, VINCENT LABELLA, University at Albany — Devices that utilize the spin degree of freedom rely on transport of electron spin through materials and material interfaces. Further knowledge of spin-polarized electron transport can aid in the development of spintronic devices. To this end, we developed a novel technique; spin polarized ballistic electron emission microscopy (SP-BEEM). This technique has been utilized to study the spin dependent transport properties in Fe/Si(001) Schottky diodes. The energetic dependence of the spin dependent attenuation lengths was measured. Most interestingly, it was found that the interface band structure played a prominent role in this dependence.

1This work was supported by the National Science Foundation CAREER-DMR-0349108, New York State Office of Science, Technology and Academic Research Faculty Development Program (NYSTAR-FDP-0020095), and MARCO Interconnect Focus Center.

4:54PM W12.00013 Spin-Valve Photo-Transistor, BIQIN HUANG, IGOR ALT Feder, IAN APPELBaUM, University of Delaware — The Spin-Valve Photo-Transistor is a semiconductor-ferromagnetic metal multilayer-semiconductor transistor operated by photo- exciting hot electrons in the emitter semiconductor into a Schottky collector. We have realized this device using a vacuum- bonded float-zone Si/multilayer/n-InP structure. To distinguish the emitter interband-excited component of collector current from base/collector internal photoemission, we use a lockin spectroscopy sensitive only to the magnetocurrent. Our experimental results indicate a pathway to improve the magnetocurrent of a related device, the Spin- Valve Photo-Diode, by increasing the fraction of hot electron current that travels through both layers of the ferromagnetic spin-valve.

5:06PM W12.00014 Influence of Spin-Orbit Interactions on Point Contact Andreev Reflection. IGN GARATE, ALLAN MACDONALD, University of Texas at Austin — In PCAR (point contact Andreev reflection) the I(V) characteristics of an interface between a singlet superconductor and a ferromagnetic metal is used (1)(2) to probe the degree of spin-polarization near the Fermi energy of the ferromagnet. Motivated by recent PCAR studies (2)(4) of (III,Mn) ferromagnetic semiconductors, in which the spin-orbit interaction scale is comparable to the exchange energy scale, we report on a theoretical study of the effect of spin-orbit interactions on the quasiparticle current through a ferromagnet-semiconductor interface. Our theoretical analysis generalizes the Blonder-Tinkham-Klapwijk model results commonly used to interpret PCAR experiments. We find that PCAR provides a good qualitative measure of Fermi energy spin-polarization, even when the quasiparticle bands are strongly spin-orbit coupled.


5:18PM W12.00015 Zero-Bias Conductance Peak in Al/AIOx/Sc Tunnel Junctions. SHENG-SHIUAN YEH, JUHN-JONG LIN, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan — We have fabricated a series of Al/AIOx/Sc tunnel junctions and measured the differential conductances at low temperatures. 25-nm thick Al (99.999%) stripes were first thermally evaporated onto a glass substrate, followed by glow discharge under an O2 atmosphere, to form a thin insulating AlOx layer. Subsequently, a 60-nm thick Sc (99.9%) film was thermally evaporated across the oxidized Al stripes to form tunnel junctions of 1 mm x 1 mm. Lock-in techniques were used to measure the differential conductances dI/dV(G) of the junctions. Zero-bias conductance peaks were found in all the tunnel junctions. In particular, the magnitudes of the zero-bias conductance peaks reveal a -lnT dependence below about 30 K, which could be attributed to the electron-magnetic-impurities interactions according to the theory of Appelbaum. However, the magnetic field has only a small effect on the conductance peaks. An asymmetric term in G(V) was observed, which is strongly temperature dependent and magnetic-field insensitive. Possible explanations will be discussed.

Thursday, March 8, 2007 2:30PM - 5:30PM —
Session W13 DMP GMAG: Focus Session: Thin Films and Superlattices —
Colorado Convention Center
Korbel 4C

2:30PM W13.00001 Fabrication and Functionality of Complex Oxide Superlattices1, HIROYUKI YAMADA, Correlated Electron Research Center (CERC), National Institute of Advanced Industrial Science and Technology (AIST) — In this talk, we focus on three-constituent magnetic oxide superlattice (‘tricolor’ superlattice), where the asymmetric stacking leads to ABCABC – artificially breaks the space-inversion symmetry. The purpose of the study is to realize artificial polar ferromagnets. The polar/noncentrosymmetric magnets, represented by multiferroic compounds, recently attract a considerable interest, because we can expect novel phenomena, such as magneto-electric (ME) effect, or magnetization-induced second harmonic generation (MSHG). In the artificial superlattice, the gigantic MSHG was first realized with a ‘tricolor’ consisting of a ferromagnet La0.5Sr0.5MnO3 and band insulators LaAlO3 (LAO) and SrTiO3 [H. Yamada et al., APL 81, 4793 (2002), Y. Ogawa, et al., PRL 90, 217403 (2003)]. From the temperature dependence of MSHG in this superlattice, we found that the MSHG originate from the interface magnetism. By utilizing the MSHG as a probe for interface magnetism, we optimized the various oxide interfaces, leading to the discoveries of huge tunneling magnetoresistance in a junction with engineered interfaces [H. Yamada et al., Science 305, 646 (2004)]. In those functionalities, crucial roles are played by the interface effects characteristic of correlated electron oxides, such as charge transfer or orbital state-mediated magnetism [H. Yamada, et al., APL89, 052506 (2006)].

1This work was done in collaboration with Tokura projects, Exploratory Research for Advanced Technology (ERATO), Japan Science and Technology Corporation (JST), and partly conducted in Core Research for Evolutional Science and Technology (CREST), JST.
3:06PM W13.00002 Physical properties of epitaxial n-type La$_{0.7}$Ce$_{0.3}$MnO$_3$ films. HSIUNG CHOU, C. Y. WU, C. B. WU. Department of Physics and Center for Nanoscience and Nanotechnology, National Sun Yat-sen University — Electronic doped Colossal Magnetoresistance (CMR) Materials have been long for spintronic applications. Since the n-type CMR material can exist only in a metastable state rather than in a thermodynamic equilibrium state [1], in situ growth of epitaxial films is regarded as an efficient way for forming single n-type CMR films. In this study, La$_{0.7}$Ce$_{0.3}$MnO$_3$ (LCeMO) films were grown on LaAlO$_3$ and SrTiO$_3$ substrates at various growth conditions. Earlier reports of LCeMO films exhibit a single $T_c$, the metal-insulator like transition temperature, at 250K. It is found in our studies, all films shows higher $T_c$ and $T_C$ between 260 and 300K. Hall measurements indicate, only specific growth conditions within a narrow growth window can approach to the metastable state and results in n-type LCeMO films. Because the Ce and La are next to each other in the periodic table, it is not easy to identify the composition of films by either the energy dispersion spectrum or the Rutherford backscattering spectrum. We are unable to tell the exact compositions of our films. The phase separation that usually occurred when the films approaches to a thermodynamic equilibrium state does not happen for our films. The detail of our results will be reported in the presentation. Reference [1]: H. Chou, C. B. Wu, S. G. Hsu, and C. Y. Wu, Phys. Rev. B 74, 174405 (2006).

3:18PM W13.00003 Influence of B-site cationic ordering on the magnetic properties of La$_2$NiMnO$_6$ epitaxial thin films. A. VENIMADHAV, D.A. TENNE, M.J. WILSON, P. SCHIFFER, QI LI, J.H. LEE, D.G. SCHLOM, X.X. XI, Penn State University — Monoclinic (0 0 1)-oriented La$_2$NiMnO$_6$ thin films were grown on (0 0 1) SrTiO$_3$ and (0 0 1) LAST substrates by pulsed-laser deposition. The crystal structures, magnetic properties, and the Raman spectrum have been studied for films with different growth conditions. The magnetic properties were found to be very sensitive to the growth conditions and to the substrate. Analysis of the magnetization, x-ray diffraction, and the Raman spectroscopy measurements demonstrate that the B-site cationic ordering, which is sensitive to both the growth conditions and the lattice mismatch with the substrate, affects the magnetic properties.

3:30PM W13.00004 Structural and Magnetic Characterization of Fe-doped La$_{2/3}$Ca$_{1/3}$MnO$_3$ Films. OSCAR LUIS ARNACHE OLMOS, Universidad de Antioquia, AXEL HOFFMANN, MSD, Argonne National Laboratory, DORIS A. GIRA LOZANO, Universidad de Antioquia — We have investigated pure and Fe-doped La$_{2/3}$Ca$_{1/3}$MnO$_3$ thin films, which were prepared via high O$_2$-pressure (500 mTorr) by magnetron DC sputtering on (100) LaAlO$_3$, (100) SrTiO$_3$ and (100) MgO substrates. The Fe-doped samples contained 1% and 3% Fe per Mn. The structural and magnetic properties of the films and targets were characterized using X-ray diffraction(XRD) and reflectivity, Mössbauer spectroscopy and magnetometry measurements. XRD shows that films are single phase and epitaxially oriented, and have negligible structural changes upon Fe-doping. The Mössbauer spectra measured at room temperature exhibit one doublet with an isomer shift of 0.320 mm/s, indicating the presence of the Fe$^{3+}$ ion at room temperature in the sample, which is a typical value of the high-spin of Fe$^{3+}$. The quadrupole splitting value was 0.210±0.006 mm/s. This clearly indicates that Fe is incorporated into the structure by substituting Mn. We will furthermore discuss the influence of Fe-doping on magnetic and magnetotransport properties.

Work supported by COLCIENCIAS and DOE.

3:42PM W13.00005 Electrical Transport and Magnetic Behavior of Pr$_{0.5}$Ca$_{0.5}$MnO$_3$ Film grown by Chemical Solution Deposition technique. M. JAIN, Q.X. JIA, Superconductivity Technology Center, MPA, Los Alamos National Laboratory, Los Alamos, NM, F. RONNING, T. PARK, J.D. THOMPSON, Condensed Matter and Thermal Physics, Los Alamos National Laboratory, Los Alamos, NM — Rare-earth manganites (R$_{1-x}$A$_x$MnO$_3$; R = rare earth, e.g. La, Pr, A = alkaline earth metal, e.g. Ca, Sr) have attracted much interest because of their rich phenomena like colossal magnetoresistance and charge ordering (CO). For certain values of $x$, close to 0.5, these compounds undergo a first-order CO transition. The CO state is characterized by the real space ordering of Mn$^{3+}$/$\text{Mn}^{4+}$ in the mixed valent manganite. The CO in bulk Pr$_{1-x}$Ca$_x$MnO$_3$ has been widely studied, however, there are very limited studies on thin films of this material. In this work, we have systematically studied the magnetic and electrical behaviors of the Pr$_{0.5}$Ca$_{0.5}$MnO$_3$ (PCMO) thin films grown by chemical solution deposition technique on LaAlO$_3$ substrates. The ground state in PCMO was found to be a charge-ordered antiferromagnetic insulator. The CO transition at 235 K was observed. With the application of magnetic field the resistivity of the film decreased at low temperatures. Detailed magnetic and electrical properties of these films will be presented.

3:54PM W13.00006 Characterization of Anisotropy in Manganite (LPCMO) Thin Films. G. SINGH-BHALLA, S. TONGAY, T. DHAKAL, R. RAIRIGH, A. BISWAS, A.F. HEBARD, University of Florida — Resistance measurements on thin films of strongly correlated electronic materials that have anisotropic properties due to atomic layering and/or substrate induced strain are primarily sensitive to in-plane conduction paths and therefore fail to capture any information about perpendicular transport. We present an experimental technique in which the films under investigation, pulse laser deposited (La$_{1-x}$Pr$_x$)$_{1/3}$Ca$_{2/3}$MnO$_3$ (LPCMO) with thicknesses in the range 300-900 Å, comprise the base electrodes of trilayer capacitor structures, thus allowing the simultaneous characterization of dc transport (resistance) in the parallel direction and ac transport (capacitance) in the perpendicular direction. For a given film, we find two distinct direction-dependent insulator-metal percolation transitions reflecting the competition between insulating and ferromagnetic metallic phases. With increasing thickness, the temperature difference between these transitions decreases. This decrease occurs because the presence of a strain-stabilized ferromagnetic metal phase at the LPCMO/substrate (NdGaO$_3$) has less of an effect on transport as the thickness increases and the LPCMO manifests isotropic bulk behavior.

4:06PM W13.00007 Plasmon Enhancement of Photoinduced Resistivity Changes in Bi$_{1-x}$Ca$_2$MnO$_3$ Thin Films. VERA SMOLYANINOVA, E. TALANOVA, RAJESWARI KOLAGANI, G. YONG, R. KENNEDY, M. STEGER, K. WALL, Towson University — Doped rare-earth manganese oxides (manganites) exhibit a wide variety of physical phenomena due to complex interplay of electronic, magnetic, orbital, and structural degrees of freedom and their sensitivity to external fields. A photoinduced insulator to conductor transition in charge-ordered manganites is especially interesting from the point of view of creating photonic devices. Thin films of Bi$_{1-x}$Ca$_2$MnO$_3$ exhibit large photoinduced resistivity changes associated with melting of the charge ordering by visible light [1]. We have found a considerable increase of the photoinduced resistivity changes in the Bi$_{1-x}$Ca$_2$MnO$_3$ thin film after depositing metal nanoparticles on the surface. This increase can be explained by enhancement of local electromagnetic field in the vicinity of the gold nanoparticle due to the plasmon resonance. The changes in lifetime of the photoinduced state will be reported, and the possible origin of these effects will be discussed. Reference [1]: V. N. Smolyaninova at al., Appl. Phys. Lett. 86, 071922 (2005).

This work is supported by NSF grant DMR-0348939.
Monitor for the Linac Coherent Light Source (LCLS) Free Electron Laser (FEL). G. YONG, R. KOLAGANI, R. MUNDELE, A. DAVIDSON, TOWSON U., Y. LIANG, Motorola Lab, O. DRURY, E. ABLES, S. FRIEDRICH, LLNL — We are developing a CMR based bolometric \( \kappa \)-ray detector as a total energy monitor for the LCLS FEL to be built at the Stanford Linear Accelerator Center. The FEL will produce \( \sim 200 \) femtosecond pulses in the energy range 0.8 to 8 keV with \( 10^{12} \) photons per pulse. The bolometer is designed to measure the total energy of each laser pulse with repeatability below 1\% and an accuracy below 10\%.

The detector is fabricated using epitaxial thin films of \( \text{Nd}_{0.67}\text{Sr}_{0.33}\text{MnO}_3 \) grown on Si by Pulsed Laser Deposition. An epitaxial buffer layer of \( \text{SrTiO}_3 \) is used as a chemical barrier and an additional template layer of \( \text{Bi}_4\text{Ti}_3\text{O}_{12} \) is employed to facilitate lattice match with the \( \text{Nd}_{0.67}\text{Sr}_{0.33}\text{MnO}_3 \) layer. We have been able to obtain good quality epitaxial thin films by this approach. Prototype detectors have been fabricated photolithographically, and are operated in a pulse tube refrigerator at temperatures between 100 to 150 K. Initial tests with a thermal heater pulse show that the film properties are sufficient for detector functionality. We will discuss the details of material optimization, characteristics of the sensor material such as the temperature coefficient of resistance and \( 1/f \) noise, and projections of the detector response under photon illumination.

4:30PM W13.00009 Observing Metal-Insulator Transitions in Spatially-Confined Perovskite Manganite Thin Films\(^1\) T. ZAC WARD, Oak Ridge National Laboratory and The University of Tennessee, H.Y. ZHAI, J.X. MA, Oak Ridge National Laboratory, KENJI FUCHIGAMI, E/WARD PLUMMER, JIAN SHEN, Oak Ridge National Laboratory and The University of Tennessee — Transition metal oxides (TMO) exhibit a strong spin-charge-lattice interaction that can lead to electronic phase separation (PS). This phenomenon carries a number of fascinating electronic and magnetic phases while maintaining a single crystalline structure. To better understand the nature of phase transition involving the coexistence of multiple phases, we have fabricated \( \text{La}_{x/8}\text{Pr}_x\text{Ca}_{9/8}\text{MnO}_3 \) (LPCMO) wires from single crystal LPCMO thin films using optical and E-beam lithographic techniques. These wires display giant and ultrasharp steps with varying temperature and magnetic field near the metal-insulator transition, which is believed to be a direct consequence of the influence of spatial confinement on percolative transport in these structures.

\(^1\)Research sponsored by the U. S. Department of Energy under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed by UT-Battelle, LLC.

4:42PM W13.00010 Low-Electric-Field Tuned Mobile Carrier Density and Heat Conduction in \( \text{SrMnO}_3 \)\(^1\) JOSHUA COHN, CORNELIU CHIORESCU, University of Miami, JOHN NEUMEIER, Montana State University — Nominally undoped \( \text{CaMnO}_3 \) (CMO) and \( \text{SrMnO}_3 \) (SMO), both G-type antiferromagnets with orthorhombic and cubic structure, respectively, exhibit very different low-temperature thermal conductivities \( (\kappa) \), with \( \kappa_{\text{CMO}} > \kappa_{\text{SMO}} \). These compounds are lightly electron doped due to oxygen vacancies, with \( n \sim 10^{18} - 10^{19} \text{ cm}^{-3} \) at room temperature. Measurements of the electrical conductivity and Hall coefficient indicate that the low-temperature mobile carrier density in SMO is larger by four orders of magnitude than that of CMO, suggesting that the disparity in \( \kappa \) values reflects enhanced phonon-electron scattering in the former compound. We will report results of thermal conductivity measurements on SMO designed to test this hypothesis by using applied electric fields to vary the mobile carrier density at fixed temperature.

\(^1\)This material is based upon work supported by the National Science Foundation under grants DMR-0072276 (Univ. Miami) and DMR-0504769 (Montana State Univ.).

4:54PM W13.00011 Low-Electric-Field Tuned Impurity Conduction in Antiferromagnetic Manganites\(^1\) CORNELIU CHIORESCU, JOSHUA COHN, University of Miami, JOHN NEUMEIER, Montana State University — Transport measurements for temperatures in the range 4.2 \( K \leq T \leq 300 \text{ K} \) are reported for the semiconducting, antiferromagnetic manganites \( \text{SrMnO}_3 \) and \( \text{CaMnO}_3 \). At low \( T \) where impurity conduction predominates, the electrical conductivity and Hall coefficient are found to be strongly electric-field dependent. For \( \text{SrMnO}_3 \), the mobile carrier density is continuously tunable over a range of more than three orders of magnitude in electric fields \( F \leq 50 \text{ V/cm} \). The conductivity and carrier density scale with field \( \propto \exp(\sqrt{F}) \), indicating Poole-Frenkel field-assisted ionization of bound carriers. The binding energy for \( \text{SrMnO}_3 \) (\( \sim 3.5 \text{ meV} \)) implies that electrons are ionized to more mobile states within the energy gap, rather than to the conduction band. This small energy scale correlates with the low-temperature onset of a small ferromagnetic moment in this compound, suggesting that bound electrons form ferromagnetic polarons. Strong electron correlation effects are suggested by the electric-field dependent Hall mobility.

\(^1\)This material is based upon work supported by the National Science Foundation under grants DMR-0072276 (Univ. Miami) and DMR-0504769 (Montana State Univ.).

5:06PM W13.00012 Voltage-induced Metal-Insulator Transitions in Perovskite Oxide Thin Films Doped with Strongly Correlated Electrons YUDI WANG, SOO GIL KIM, I-WEI CHEN, University of Pennsylvania — We have observed a reversible metal-insulator transition in perovskite oxide thin films that can be controlled by charge trapping pumped by a bipolar voltage bias. In the as-fabricated state, the thin film is metallic with a very low resistance comparable to that of the metallic bottom electrode, showing decreasing resistance with decreasing temperature. This metallic state switches to a high-resistance state after applying a voltage bias: such state is non-ohmic showing a negative temperature dependence of resistance. Switching at essentially the same voltage bias was observed down to 2K. The metal-insulator transition is attributed to charge trapping that disorders the energy of correlated electron states in the conduction band. By increasing the amount of charge trapped, which increases the disorder relative to the band width, increasingly more insulating states with a stronger temperature dependence of resistivity are accessed. This metal-insulator transition provides a platform to engineer new nonvolatile memory that does not require heat (as in phase transition) or dielectric breakdown (as in most other oxide resistance devices).

5:18PM W13.00013 Variable electron correlation in high-quality MBE- and PLD-grown \( \text{SrRuO}_3 \) thin films. WOLTER SIEMONS, GERT JAN KOSTER, Stanford University, HIDEKI YAMAMOTO, NTT Basic Research Laboratories, ARTURAS VAILIONIS, THEODORE GEBALLE, Stanford University, DAVE BLANK, University of Twente, MALCOLM BEASLEY, Stanford University — We show that systematic variations in the degree of electric fields can occur within \( \text{SrRuO}_3 \) as a function of disorder/off-stoichiometry. In particular, we find that one source of disorder can be controlled in \( \text{SrRuO}_3 \) thin films by varying the deposition conditions or the deposition technique. Specifically, we clearly demonstrate that variation of vacancies on the ruthenium site gives rise to a variation in correlated behavior as seen in the photoemission spectra (XPS and UPS). Moreover, the transport properties of our samples are clearly linked to their photoemission spectra, and independently the crystal unit cell parameters. \( \text{SrRuO}_3 \) appears to be a system where these effects can be studied in a more systematic fashion, usually not easily accessible, but we suspect that the underlying physics is generic in complex oxidesWork supported by the DoE BES and EPRI.
2:30PM W14.00001 Magnetic Properties of Epitaxial Cr/Cr$_2$O$_3$/ Cr Multilayers$^1$, TATHAGATA MUKHERJEE, SARBESWAR SAHOO, CHRISTIAN BINEK, University of Nebraska-Lincoln — We study Cr/Cr$_2$O$_3$/Cr trilayer structures grown by Molecular Beam Epitaxy on (111) oriented Al$_2$O$_3$ substrates. X-ray diffraction reveals perfect single crystalline (110) Cr and stoichiometric single crystalline Cr$_2$O$_3$ (111) films. Both, Cr and Cr$_2$O$_3$ order antiferromagnetically with bulk Néel temperatures of 311 and 307K, respectively. Cr is an itinerant antiferromagnet where the antiferromagnetic (AF) order establishes as an incommensurate spin density wave. Cr$_2$O$_3$ in contrast is an AF insulator with localized magnetic moments where magnetoelectric and piezomagnetic effects are both symmetry allowed. Its insulating, magnetoelectric and piezoelectric properties make Cr$_2$O$_3$ an interesting material for extrinsically controlled tunnel barriers in TMR type structures. The lattice mismatch of $\sim$1.2% at the Cr – Cr$_2$O$_3$ interface creates a strong stress induced piezomagnetic moment revealed by SQUID measurements. The interaction between the piezomoment and the spin distribution at the Cr interface gives rise to a rich scenario of magnetic proximity effects which we study by SQUID magnetometry, magneto-optical Kerr effect and electrical transport measurements.

$^1$Financial support by NCSER and NRI is gratefully acknowledged.

2:42PM W14.00002 Piezomagnetism in Epitaxial Cr$_2$O$_3$ Thin Films$^1$, YI WANG, SARBESWAR SAHOO, CHRISTIAN BINEK, University of Nebraska-Lincoln, BINEK TEAM — Recently, the magnetoelectric material Cr$_2$O$_3$ attracted renewed interest due to its potential for future spintronics applications which can be realized by novel magnetic thin film heterostructures$^1$. Here we study thin films of Cr$_2$O$_3$ (111) on c-Al$_2$O$_3$ (111) substrate which are grown by thermal evaporation of Cr metal in an O$_2$ atmosphere. X-ray diffraction data reveal stoichiometric epitaxially grown Cr$_2$O$_3$ (111) films. Owing to a lattice mismatch of $\sim$4% at the interface between the Al$_2$O$_3$ substrate and the film we observe a strong stress induced piezomagnetic moment in the Cr$_2$O$_3$ film. We measure the temperature dependence of this piezomoment by Superconducting Quantum Interference Device (SQUID) magnetometry and Kerr rotation. The presence of high inherent stress, a significant piezomagnetic moment and the possibility to realize high electric fields makes our Cr$_2$O$_3$ thin films ideal candidates for the challenging quest of the symmetry allowed but hitherto undiscovered piezomagnetoelectric effect. [1] Ch. Binek, B. Doudin, J. Phys. Condens. Matter 17, L39 (2005).

$^1$Financial support from the NSF through Career DMR-0547887, NRI and the NSF MRSEC DMR-0213808 is gratefully acknowledged.

2:54PM W14.00003 Magnetoelectric thin films for electrically controlled exchange bias in spintronic applications$^1$, XI HE, SARBESWAR SAHOO, SRINIVAS POLISETTY, YI WANG, TATHAGATA MUKHERJEE, CHRISTIAN BINEK, University of Nebraska-Lincoln — Epitaxial (111) oriented films of magnetoelectric (ME) Cr$_2$O$_3$ are grown by MBE. These films are the key component of Cr$_2$O$_3$(111)/Co/Pt$_3$ heterostructures allowing for electrically controlled exchange bias (EB) and novel spintronic applications$^1$. Pure voltage control of magnetic configurations in TMR-type devices is proposed as an alternative to current-induced switching. Basic effects of electrically controlled EB and its ME switching are studied by magnetometry and polar Kerr rotation. Exchange coupling between the ME antiferromagnet Cr$_2$O$_3$ and the ferromagnetic CoPt multilayer gives rise to perpendicular EB. The latter is controlled by axial electric fields inducing excess magnetization at the interface which controls the EB field. Recently, the sign of the EB field has been tuned via a field cooling procedure where a Cr$_2$O$_3$(111)/Co/Pt$_3$ system is exposed to either parallel or antiparallel axial magnetic and electric fields$^2$. Here we study this ME switching effect in an all thin film heterostructure. [1] Ch. Binek, B. Doudin, J. Phys. Condens. Matter 17, L39 (2005). [2] P. Borisov et al., Phys. Rev. Lett. 94, 117203 (2005).

$^1$Supported by NSF through Career DMR-0547887, MRSEC and NRI.

3:06PM W14.00004 Coupling Magnetism to Electricity in Multiferroic Heterostructures$^1$, RAMAMOOPTHY RAMESH, University of California, Berkeley — Complex perovskite oxides exhibit a rich spectrum of functional responses, including magnetism, ferroelectricity, highly correlated electron behavior, superconductivity, etc. The basic materials physics of such materials provide the ideal playground for interdisciplinary scientific exploration. Over the past decade we have been exploring the science of such materials (for example, colossal magnetoresistance, ferroelectricity, etc.) in thin film form by creating epitaxial heterostructures and nanostructures. Among the large number of materials systems, there exists a small set of materials which exhibit multiple order parameters; these are known as multiferroics. Using our work in the field of ferroelectric (FE) and ferromagnetic oxides as the background, we are now exploring such materials, as epitaxial thin films as well as nanostructures. Specifically, we are studying the role of thin film growth, heteroepitaxy and processing on the basic properties as well as magnitude of the coupling between the order parameters. In our work we are exploring the switchability of the antiferromagnetic order using this coupling. What is the importance of this work? Antiferromagnets (AFM) are pervasive in the recording industry. They are used as exchange biasing layers in MTJ’s etc. However, to date there has been no antiferromagnet that is electrically tunable. We believe that the multiferroic BiFeO$_3$ is one compound where this can be observed. The next step is to explore the coupling of a ferromagnet to this antiferromagnet through the exchange biasing concept. Ultimately, this will give us the opportunity to switch the magnetic state in a ferromagnet (and therefore the spin polarization direction) by simply applying an electric field to the underlying antiferromagnetic ferroelectric. In this talk, I will describe our progress to date on this exciting possibility.

$^1$This work is supported by the US Department of Energy and the Office of Naval Research.

3:42PM W14.00005 Coercivity and Nano-structure in Magnetic Spinel Mg(Mn,Fe)$_2$O$_4$, CHENGLIN ZHANG, S. YEO, S.-W. CHEONG, Department of Physics & Astronomy, Rutgers University, Piscataway, New Jersey 08854, Y. HORIBE, S. MORI COLLABORATION$^1$, C. M. TSENG, C. H. CHEN COLLABORATION$^2$ — We discovered that the micro-to-nano-structure of Mg(Mn,Fe)$_2$O$_4$ drastically changes with different thermal treatment. This extraordinary structural evolution is associated with spinodal chemical decomposition associated with the Jahn-Teller structural distortions around Mn ions. The magnetic properties of the polycrystalline Mg(Mn,Fe)$_2$O$_4$ vary with the structural progress. Particularly, the Curie temperature and magnetic coercivity change with the structural evolution. The significantly-enhanced coercivity in the system with elongated nanostucture stems from the large shape anisotropy of the nanostructure.

$^1$Dept. of Physics, Osaka Prefecture Univ, Japan

$^2$Center for Condensed Matter Sciences, National Taiwan University, Taiwan
3:54PM W14.00006 Magnetic Properties of Cobalt-Ferrite Nanoparticles Prepared by a Sol-Gel Synthesis Technique1 THOMAS EKIERT, KARL UNRUH, University of Delaware, E. CARPENTER, Virginia Commonwealth University, K. PETTIGREW, J. LONG, D. ROLISON, Naval Research Laboratory — Cobalt-ferrite nanoparticles have been prepared as highly porous aerogels using a sol-gel technique and characterized by XRD, TEM, and nitrogen-sorption porosimetry measurements. The XRD patterns for calcined Co-ferrite aerogels corresponded to a cubic structure with a lattice parameter near that of bulk Co-ferrite and a particle size of about 6 nm. TEM images indicated a similar particle size and a morphology similar to that of silica aerogels. The magnetic properties of these materials have been studied from 5 K to 340 K. Hysteresis loop measurements indicated that the coercivity and saturation magnetization of these materials evolves from nearly 19 kOe and 56 emu/g at 5 K to less than 10 Oe and 40 emu/g at 340 K. ZFC magnetization curves displayed a broad maximum that smoothly varied between about 300 K in an applied field of 100 Oe to about 180 K in a 10 kOe field. These measurements have been interpreted in terms of a distribution of effective particle sizes arising from a distribution in interparticle interactions.

1This work has been supported in part by ARO DEPSCOR grant no. W911NF-04-1-0264.

4:06PM W14.00007 Investigations of a New Diluted Magnetic Oxide with Room Temperature Ferromagnetism in Co-doped HfO2 Y.H. CHANG, W.C. LEE, M.L. HUANG, Dept. of Materials science and Engineering, National Tsing Hua Univ., Taiwan, S.F. LEE, Inst. of Physics, Academia Sinica, Taiwan, T.Y. SOO, Dept. of Physics, National Tsing Hua Univ., Taiwan, M. HONG, Dept. of Materials science and Engineering, National Tsing Hua Univ., Taiwan, J. KWÓ, Dept. of Physics, National Tsing Hua Univ., Taiwan — The structural, chemical, and magnetic properties of HfO2 epitaxial films ~100nm thick grown on YSZ at varying growth temperature have been systematically investigated. Nearly cobalt cluster-free films with RT ferromagnetic behaviors can be obtained via low T growth. In-situ XPS analysis during growth indicated the formation of metallic cobalt at the initial growth stage under a low O2 partial pressure ~10^−10 Torr, and that the metallic cobalt can be mostly eliminated by raising the pressure to 10^−7 Torr. In conjunction with EXAFS local structural analysis and post annealing experiments, we infer that cobalt ions in low T grown films are located at interstitial site and appear to be stable after being annealed in O2 at 350°C. Further Hall measurements are now underway to measure the carrier concentration, and to elucidate their role to the apparent ferromagnetism.

4:18PM W14.00008 Magnetocaloric effect (MCE) in Nickel Ferrite nanoparticles J. GASS, M.B. MORALES, N.A. FREY, M.J. MINER, S. SRINATH, H. SRIKANTH, University of South Florida — We report on the magneto caloric effect (MCE) in a Nickel ferrite (NiFe2O4) nanoparticle system. The nanoparticles were synthesized using chemical co-precipitation. Extensive characterization of structural and magnetic properties was done using XRD, TEM, DC and AC magnetization, and transverse susceptibility. The change in entropy was calculated using the thermodynamic Maxwell relation from the family of M-H curves taken at different temperatures. Maximum entropy change in nanoparticle systems is influenced by particle size, anisotropy, and collective dipolar behavior. While the MCE is not as large as that reported in bulk systems, there are advantages as ferrite nanoparticles are easily produced and the operational temperature is tuned by the average particle size. In our studies, we observed a sharp peak in M-T curves by particle size, anisotropy, and collective dipolar behavior. While the MCE is not as large as that reported in bulk systems, there are advantages as ferrite nanoparticles are easily produced and the operational temperature is tuned by the average particle size. In our studies, we observed a sharp peak in M-T curves at around 60K in addition to the blocking transition which occurs at 120 K. This results in a larger entropy change in comparison with the MCE results on other reported ferrite nanoparticles. The origin of this anomalous MCE is analyzed in the context of surface anisotropy and other possible contributions in the NiFe2O4 system. Work supported by NSF through grant CTS-0408933.

4:30PM W14.00009 Verwey transition and magnetic irreversibility in nano-crystalline maghemite produced by magnetotactic bacteria T. PROZOROV, Ames Laboratory, R. PROZOROV, Ames Laboratory and Department of Physics & Astronomy, Iowa State University, Ames IA, T.J. WILLIAMS, Ames Laboratory, Ames IA, D.A. BAZYLNISKI, School of Life Sciences, University of Nevada, Las Vegas, NV, S.K. MALLAPRAGADA, Ames Laboratory and Department of Chemical and Biological Engineering, Iowa State University, Ames IA, B. NARASIMHAN, Department of Chemical and Biological Engineering, Iowa State University, Ames IA — Magnetic properties of 50 nm maghemite nanocrystals from different strains of magnetotactic bacteria are compared to high quality single crystal. It is found that the Verwey transition depends mostly on the particle shape. It is sharp and occur at a temperature approaching bulk values in elongated nanoparticles from M. baltanica. This result contradicts previous reports of the Verwey temperature reduction in nanoparticles. Magnetic irreversibility below the Verwey transition shows thermal-history dependence and, in nanoparticles, is strongly influenced by the interparticle interactions. Collected data are analyzed in terms of the interplay between crystalline and shape anisotropies as well as collective behavior of the nanoparticles.

4:42PM W14.00010 Magnetic properties of Fe3O4 and CoFe2O4 ferrofluids M.B. MORALES, J. GASS, S.L. MORROW, H. SRIKANTH, Department of Materials Science and Engineering, University of South Florida — We study in detail the magnetic properties of ferrofluids consisting of ~0.02 g/cm³ volume concentration of surfactant Fe3O4 and CoFe2O4 nanoparticles suspended in two solvents, hexane and dodecane, with different room temperature viscosities. DC and AC magnetization measurements were done using a Physical Properties Measurement System (PPMS). Hysteresis loops of Fe3O4 in both liquids at different temperatures show that the particles are superparamagnetic having low coercivities even at low temperature. CoFe2O4-based ferrofluids, on the other hand, have a wide range of grain sizes and show high coercivity of 10 kOe at low temperature. From the ZFC-FC curves, the blocking temperature was determined to be 76 K and 223 K for Fe3O4 and CoFe2O4 in dodecane, respectively. To probe the dynamic relaxation effects, temperature-dependent complex AC susceptibility of all the ferrofluids were measured at frequencies of 100 Hz and 10 kHz. From these data sets, the relaxation contributions due to Neel and Brownian mechanisms were identified. We will also report on systematic magnetic measurements and analysis of ferrofluids with different nanoparticle concentrations.

4:54PM W14.00011 Quantum Monte-Carlo Study of Mn and Mn-oxide clusters HIORI KINO, LUCAS K. WAGNER, LUBOS MITAS, Department of Physics, North Carolina State Univer., NATIONAL INSTITUTE FOR MATERIALS SCIENCE, JAPAN COLLABORATION — Many molecules and clusters of Mn and Mn-oxide have not only interesting physical properties but also can be found in enzymes as important components in biochemical reactions. The electronic structure calculations of these systems are difficult and, for example, choice of exchange-correlation functionals in Density Functional Theory can significantly influence both ground state geometries and spin-state predictions. Therefore, highly accurate calculation is very desirable for these systems. Experimentally, it is established that the Mn dimer is a van der Waals system with weak binding, however, the spin multiplicity has not been settled unambiguously with possibilities covering a range from singlet, triplet, etc, up to 2S+1=11. On the other hand, MnMO4-based clusters are quite well understood as being a high-spin system, but their geometries depend on the exchange-correlation functionals. We will present results from our calculations and compare them to results from the fixed-node quantum Monte Carlo calculations of these systems. We will also report on recent progress in modeling the [Mn4O-4Ca] cluster structural prototypes for the oxygen evolving center in green plants Photosystem II.

5:06PM W14.00012 Magnetic Isomerization of Chromium Clusters WEI JIANG, FORREST PAYNE, LOUIS BLOOMFIELD — We have used the Stern-Gerlach deflection technique to study magnetic properties of chromium clusters of different sizes (N=20-133) at different temperatures (T=60K-120K) and magnetic fields. Though chromium bulk is antiferromagnetic, we observed that nearly all these clusters are magnetic. And the deflection profiles of them suggest that two or more magnetic isomers exist in the beam, which have significantly different magnetic moments.

1This material is based upon work supported by NSF under Grant No. DMR-0405203.
5:18PM W14.00013 Simulation of interacting nanoparticles with random anisotropy axes, JULIO F. FERNANDEZ, CSIC, Zaragoza, Spain, JUAN J. ALONSO, Universidad de Malaga, Spain — We report Monte Carlo simulation results for the collective behavior of single-domain nanoparticles with randomly oriented easy magnetization axes. Such randomness may follow from a random orientation of the crystalline axes within each nanoparticle. Dipole-dipole interactions, as well as nearest neighbor exchange interactions of various strengths are taken into account. We report on the effect random anisotropy has on long range order as well as on magnetic relaxation at low temperature.

Thursday, March 8, 2007 2:30PM - 5:06PM
Session W16 GMAG DCOMP DMP: Focus Session: Theory of Magnetism: Traditional and Novel Magnets Colorado Convention Center Korbel 4F

2:30PM W16.00001 Exact Diagonalization studies of frustrated AFM Heisenberg polytopes, IOANNIS ROUSOCHATZAKIS, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne (EPFL), ANDREAS LAECHL, Institut Romand de Recherche Numerique en Physique des Matériaux (IRRMA), EPFL, FREDERIC MILA, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne (EPFL) — We explore the low energy physics of the AFM $s = 1/2$ Heisenberg model on a number of frustrated magnetic molecule systems using exact diagonalization (ED). Particular emphasis is given to molecules with spins occupying the vertices of symmetric polyhedra. To this end, we have extended the standard ED technique in order to exploit the full point group (permutation) symmetry, thus including higher than one-dimensional irreducible representations. Apart from calculating the energy spectra according to both spin and permutation symmetries, our method provides the exact level degeneracies. In particular, for large frustrated polytopes, we find the existence of an accordingly large number of low-lying singlets below the first triplet, similarly to the case of frustrated 2D magnets. We also study the properties of the local spectral density functions, in view of interpreting recent neutron scattering experiments in Fe$_{30}$, one of the biggest AFM frustrated molecule available (comprising 30 spins 5/2 mounted on the vertices of aicosidodecahedron).

2:42PM W16.00002 Phase Oscillations of the Kondo Effect in Single-Molecule Magnets, MICHAEL N. LEUENBERGER, NanoScience Technology Center and Department of Physics, University of Central Florida, EDUARDO R. MUCCIOLO, Department of Physics, University of Central Florida — We show that it is possible to topologically induce or quench the Kondo resonance in the conductance of a single-molecule magnet ($s > 1/2$) strongly coupled to metallic leads. This can be achieved by applying a magnetic field perpendicular to the molecule easy axis and works for both full- and half-integer spin cases. The effect is caused by the Berry-phase interference between two quantum tunneling paths of the molecule’s spin. We have calculated the renormalized Berry-phase oscillations of the Kondo peaks as a function of the transverse magnetic field as well as the conductance of the molecule by means of the poor man’s scaling method. We propose to use a new variety of the single-molecule magnet Ni$_4$ for the experimental observation of this phenomenon.


2:54PM W16.00003 Single-ion and exchange anisotropy in high-symmetry tetramer single molecule magnets, DIMITRI EFREMOV, Technische Universitaet Dresden, RICHARD KLEMM, Kansas State University — We study the effects of single-ion and both symmetric and antisymmetric exchange anisotropy in equal-spin $s_1$ tetramer single molecule magnets exhibiting the molecular group symmetries $g = C_{4h}, D_{4h}, C_{2v}, D_{2d}$, and $T_d$. The near-neighbor and next-nearest-neighbor isotropic exchange interactions are $J$ and $J'$, respectively. From the vector basis used to diagonalize the general quadratic spin-spin interaction Hamiltonian $\mathcal{H}$ for each site and site pairs, we impose the symmetries characteristic of each $g$ upon $\mathcal{H}$. Using our exact, compact forms for the four-spin single-ion matrix elements, we calculate the eigenstate energies to first order in the anisotropy interactions. Type I tetramers with $J' < J > 0$ act as two dimers with maximal pair quantum numbers $s_{13} = s_{24} = s_{41}$ at low temperature $T$. Type II tetramers with $J > J' < 0$ are frustrated, with minimal low-$T$ pair quantum numbers. For both Type-I and Type-II antiferromagnetic tetramers, we calculate the first-order level-crossing inductions analytically. Accurate Hartree expressions for the thermodynamics, electron paramagnetic resonance (EPR) and inelastic neutron scattering cross-section are given. An EPR procedure to extract the effective microscopic parameters is provided.

Supported in part by the NSF through Contract No. NER-0304666.

3:06PM W16.00004 Double-Exchange Model for Molecule-Based Magnets, SERKAN ERDIN, MICHEL VAN VEENENDAAL, Department of Physics, Northern Illinois University, DeKalp, IL and Advanced Photon Source, Argonne National Laboratory, Argonne, IL — We report a detailed study of a model proposed for the molecule-based magnets, which is similar to the double-exchange mechanism. The model is applied to a two-dimensional periodic complex made of a transition metal and an organic molecule in which the electronic structure is described by effective $d$ orbitals of the transition ion at infinite Hund’s coupling limit and the lowest unoccupied molecular orbital of the organic molecule. Depending on the average electron density of the organic molecules and various superexchange couplings between metal ions’ core spins, magnetic states of the complex are investigated. In Monte-Carlo calculations for a model Hamiltonian, as a function of electron density on the organic molecule, the average magnetization and critical magnetic ordering temperatures are determined.

3:18PM W16.00005 Stripes and hysteresis in thin film ferromagnets, DAVID CLARKE, OLEG TRETIAKOV, OLEG TCHERNYSHYOV, Johns Hopkins University — Recent experimental studies have focused on the magnetic behavior of thin materials that have strong out-of-plane anisotropy. We study the behavior of such systems near the reorientation phase transition (RPT), the point at which the dipolar interaction overcomes the internal anisotropy to force the magnetization to lie in the plane. Previous studies have classified canted, polarized, and stripe domain regions of the thermodynamic phase diagram, but have not found the boundaries of metastability necessary for an understanding of observed hysteresis curves. We complete the anisotropy-applied field phase diagram near the RPT by including metastability boundaries and find the hysteresis loops characteristic of the model using analytic and numerical techniques. The system displays a line of second order transitions from a canted phase to a spin density wave (SDW) phase, and first order transitions from the SDW phase to a striped phase. We show the existence of a liquid-gas like critical point beyond which the SDW and striped phases are indistinguishable. The phase diagram is universal for thin ferromagnetic materials up to a rescaling of the applied field and effective anisotropy by a characteristic value proportional to the square of the ratio of the thickness to the exchange length. The hysteresis loops found match behavior observed in experiments. This work was supported in part by NSF Grant DMR-0524091.

3:30PM W16.00006 Stripes and Metastable Magnetization Configurations in Thin Films, ADEBANJO ORIADE, Department of Physics and Astronomy, University of Delaware, Newark DE 19716, SIU-TAT CHUI, Bartol Research Institute & Department of Physics and Astronomy, University of Delaware, Newark DE 19716 — An important aspect of the utility of magnetic tunnel junctions and the giant magneto-resistive effect devices is reversal of the magnetization of a thin film. In these devices, found in hard disk drive read heads and magneto-resistive random access memory technology, robust control of magnetization in thin films is necessary. We study, via Monte-Carlo simulations, the nature of metastable metastable magnetization states in thin films and their connection to failure in the reversal process. These metastable states usually show up as plateaus in the hysteresis loop close to the switching field. The net magnetization of the film in this state is much less than the saturation magnetization. Details of the magnetization configuration in, and during reversal of, these metastable states are presented. Two mechanisms for failure are described. (1) Strong stray fields that exist during the reversal of these metastable states will affect other elements within as much as 1µm from the longest edge of an 0.2µm × 1µm × 50Å film. (2) Turning field off whilst the film is in a metastable state results in relaxation into a paramagnetic state, useless for application.
3:42PM W16.00007 2d order ferromagnetic resonance in nanoparticles and the dating of archaeological ceramics, DEREK WALTON, McMaster Un. — Ferromagnetic resonance is almost exclusively explored experimentally in 1st order where one photon decays into a single magnon, necessarily of the uniform or magnetostatic modes. In 2d order where the photon creates two magnons of equal and opposite wave-vector, it is well-known that details of the magnon spectrum become significant. An important consideration is the cut-off in the dispersion relations for magnons whose wavelength exceeds twice the scale of the particle. I will discuss the use of this property to selectively magnetize or demagnetize assemblies of single domain grains. This permits rather sensitive dating of ancient ceramics, and accurate determination of grain size distributions.

3:54PM W16.00008 First-principles Calculation of the Single Impurity Surface Kondo Resonance, CHIUNG-YUAN LIN, IBM Almaden Research Center, San Jose, CA 95120-6099, ANTONIO CASTRO NETO, Department of Physics, Boston University, Boston, MA 02215, BARBARA JONES, IBM Almaden Research Center, San Jose, CA 95120-6099 — We have performed first-principles calculation of the surface and bulk wavefunctions of the Cu(111) surface and their hybridization energies to a Co adatom, including the potential scattering from the Co [1]. By analyzing the calculated hybridization energies, we have calculated the Kondo temperature to remarkable accuracy. We find the bulk states dominate the contribution to the Kondo temperature, in agreement with a recent experiment [2]. Furthermore, we also calculate the tunneling conductance of a scanning tunneling microscope on this system and compare our results with recent experiments of Co impurities in the Cu(111) surface. Good quantitative agreement is found at short parallel impurity-tip distances (< 6 angstroms). Our results indicate the need for a new formulation of the problem at larger distances. [1] C.-Y. Lin, A. H. Castro Neto, and B. A. Jones, Phys. Rev. Lett. 97, 156102 (2006). [2] N. Knorr, M. A. Schneider, L. Diekhoner, P. Wahl, and K. Kern, Phys. Rev. Lett. 88, 096804 (2002).

4:06PM W16.00009 Shot Noise in the SU(4) Kondo regime, VITUSHINSKIY PAVEL, Universite de Sherbrooke, Sherbrooke (QC), Canada, LE HUR KARYN, Yale University, New Haven (CT), USA, CLERK AASHISH, McGill University, Montreal (QC), Canada — It has recently been shown that shot noise is a direct probe of interparticle interactions which characterize the Fermi liquid fixed point of the standard Kondo model. We now examine the transport properties of the systems which are known to exhibit an unusual SU(4) Kondo correlated liquid behaviour at low temperatures. It was shown using T-matrix approach that conductance in this regime has unexpected linear in $eV$ corrections, as dictated by the low-energy SU(4) Fermi-liquid fixed point. We confirm this result by the microscopic calculation of backscattering current using Keldysh formalism. The SU(4) symmetry in turn affects the current shot noise and thus leads to renormalized value of the effective charge.

4:18PM W16.00010 Exact solution of SU(4) non-equilibrium Kondo model at the Toulouse point, SOLOMON DUKI, HARSH MATHUR, Case Western Reserve University — SU(4) symmetry in quantum dots has become a growing interest in both semiconductor quantum dots and carbon nanotube quantum dots[1]. We investigate theoretically the properties of an SU(4) Kondo model out of equilibrium by solving the problem exactly at a special point in the parameter space. The solution reveals that, in contrast to the SU(2) model, there are two more excitations in the system other than the charge and spin excitations. We investigate the differential conductance for arbitrary voltage bias. [1] P. Jarillo-Herrero, J. Kong, H.S.J. van der Zant, C. Dekker, L.P. Kouwenhoven and S. De Franceschi, http://www.nature.com/openurl?url_ver=Z39.88-2004&rft_val_fmt=info:ofi/fmt:kev:mtx:journal&rft.genre=journal&rft.issn=0305-461X&rft.volume=434&rft.spage=484 &rft.date=2005 (Nature) 434, 484, (2005).

4:30PM W16.00011 Spatially dependent Kondo effect in Quantum Corrals, ENRICO ROSSI, DIRK K. MORR, University of Illinois at Chicago, Chicago IL 60607. — We study the Kondo screening of a single magnetic impurity placed inside a quantum corral consisting of non-magnetic impurities on the surface of a metallic host system. We show that the spatial structure of the corral’s eigenmodes leads to a spatially dependent Kondo effect whose signatures are experimentally measurable spatial variations of the Kondo temperature, $T_K$, and of the critical Kondo coupling, $J_{cr}$. Moreover we find that the screening of the magnetic impurity is accompanied by the formation of multiple Kondo resonances with characteristic spatial patterns that provide further experimental signatures of the spatially dependent Kondo effect. Our results demonstrate that quantum corrals provide new possibilities to manipulate and explore the Kondo effect.

3 We acknowledge financial support from NSF and DOE.

4:42PM W16.00012 Propagators in Position, Momentum, and Spin Variables, BAILEY HSU, JEAN-FRANCOIS VAN HUELE, Brigham Young University — Propagators describe the evolution of quantum dynamical systems. Their expression depends on the dimension of the system, on the environment, and on the boundaries. Specific techniques have been developed to calculate the propagators for different functional forms of the potential, which in the case of spinless particles depend on position and momentum. Particles with spin interacting with magnetic fields in Stern-Gerlach-like systems lead to propagators involving position and spin variables. Spin-orbit-like systems combine momentum and spin variables. We investigate the applicability of methods found in the literature to systems that exhibit different combinations of momentum, position, and spin variables.

4:54PM W16.00013 Size Distribution of Superparamagnetic Particles Determined by Magnetic Sedimentation, JEAN-FRANCOIS BERRET, CNRS — We report on the use of magnetic sedimentation as a means to determine the size distribution of dispersed magnetic particles. The particles investigated here are i) single anionic and cationic nanoparticles of diameter D ~ 7 nm and ii) nanoparticle clusters resulting from electrostatic complexation with polyelectrolytes and polyelectrolyte-neutral copolymers. A theoretical expression of the sedimentation concentration profiles at the steady state is proposed and it is found to describe accurately the experimental data. When compared to dynamic light scattering, vibrating sample magnetometry and cryogenic transmission electron microscopy, magnetic sedimentation exhibits a unique property: it provides the core size and core size distribution of nanoparticle aggregates.

Thursday, March 8, 2007 2:30PM - 5:06PM – Session W27 DMP DCOMP: Focus Session: Computational Nanoscience IX - Nanowire, Rods & SAMs Colorado Convention Center 301

2:30PM W27.00001 ABSTRACT WITHDRAWN

2:42PM W27.00002 Conductance of telescoped double wall nanotubes calculated with ADF program package, RYO TAMURA, Shizuoka University — In double wall nanotubes (DWNts), the interlayer current is negligible compared to the intra-layer current. When the inner tube is partially extracted (telescoped) from the outer tube, however, the total current must flow between the layers so that the interlayer interaction drastically influences the conductance. Here the interlayer bonds can be considered as weak covalent bonds rather than van der Waals bonds since they are anisotropic and their number per atom is limited. In this presentation, the transfer integrals between the layers are calculated by ADF program package and their effects on the conductance in the telescoped DWNts are investigated. They are compared with our previous results.
2:54PM W27.00003 Origin of Giant Piezoresponse in Pristine $\langle 111 \rangle$-Si nanowires$^1$. JUEXIAN CAO, RUQIAN WU — It was found recently that silicon nanowires possess an unusually large piezoresponse coefficient, 350 times higher compared with Si bulk. Using first principles density functional calculations, we demonstrated that this stems from the strain-induced change in band ordering of surface states. The pristine $\langle 111 \rangle$-Si nanowire is metallic under ambient condition but the mobility of the carrier is extremely small due to the strong localization. The compression shrinks the surface shell and hence shifts the itinerant state across the Fermi level, which consequently leads a surge in conductance. The effective masses of those two bands differ by a factor of 100, a number that can roughly account the experimental data. Since the key bands for transport are surface states, the surface modification plays a vital role on the piezoresponse effects, as observed experimentally.$^1$

3:06PM W27.00004 ABSTRACT WITHDRAWN —

3:18PM W27.00005 The structure and stability of thin H-passivated $\langle 112 \rangle$ silicon nanowires, NING LUI, Iowa State University, CRISTIAN CIOBANU, Colorado School of Mines, TZU-LIANG CHAN, University of Texas at Austin, CAI-ZHUANG WANG, Ames Laboratory, KAI-MING HO, Iowa State University, FENG-CHUAN CHUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung, 804 TAIWAN — Recent experiments on the synthesis on monocrystalline nanowires reveal that their axis can only have a limited number of crystalline orientations. Among these orientations, $\langle 112 \rangle$ is the highest Miller-index wire axis and generates a rectangular cross-sectional shape. Using a combination between genetic algorithm search and density functional theory calculations, we determine the precise shape of the wire cross-section that corresponds to the lowest formation energy per silicon atom. We analyze the deviations of the cross-sectional shape from the Wulff shape, and show how the shape of the nanowires evolves as a function of cross-sectional area and the chemical potential of hydrogen.

3:30PM W27.00006 Small World Carbon Nanomaterials: Density Functional Theory Simulations$^1$. JEREMY YANCEY, MARK NOVOTNY, Dept. of Physics and Astronomy, Mississippi State University, STEVEN GWALTNEY, Dept. of Chemistry, Mississippi State University — The possible existence of small, pure carbon molecules based on physical small-world networks is addressed using density functional theory calculations. A ring of atoms with one or more small-world connections between pairs of non-nearest-neighbor sites was chosen for the network topology. The small-world connections are made with and without additional carbon atoms placed along the link. The energy per atom of these small-world carbon systems is compared with benchmark carbon clusters such as the C$_{60}$ ring, bowl, and cage isomers, the C$_{60}$ Buckyball, monocyclic pure carbon rings ranging from C$_4$ to C$_{60}$, bare linear carbon chains ranging from C$_2$ to C$_{18}$, fullerenes ranging from C$_{20}$ to C$_{60}$, and various all-carbon graphitic fragments. The energy per atom results for these materials provides an indication that some of these pure-carbon small-world nanomaterials are reasonable for real world synthesis.$^1$ Supported in part by NSF grants DMR-0426488 and DMR-0444051. Computer time from the Mississippi State University High Performance Computing Collaboratory (HPC$^2$).

3:42PM W27.00007 Electronic properties of 1D LaB$_6$ rods$^1$, G. P. LI, W. N. MEI, JING LU, R. F. SABIRIANOV, Department of Physics, University of Nebraska at Omaha, C. L. CHEUNG, X. C. ZENG, Deparment of Chemistry, University of Nebraska-Lincoln — Metal hexa-borides have varieties of interesting properties and were utilized frequently in technological applications: e.g. LaB$_6$ is known to have extremely low work function, thus is used as one of the most popular electron emitter. Our project is initiated by the experimental findings that LaB$_6$ nano-rods generated stronger electric current than in the bulk case. Thus we focus on the band structure calculations of quasi-1D nano-rods with various widths and breadths for the purpose of studying the relationship between work function and rod shapes. Our samples consist of up to ten unit cells, i.e. na X mb (a and b are lattice vectors and n X m \leq 10). To accomplish our calculations, we applied GGA density functional theory with all electron and relativistic effect included.$^1$

3:54PM W27.00008 Measuring Order and the Debye-Waller Factor for Porous Arrays, FORREST KAATZ, Owens Community College, ADHEMAR BULTHEEL, K.U.Leuven Belgium, TAKESHI EGAMI, University of TN — We derive methods that explain how to quantify the amount of order in “ordered” and “highly ordered” porous arrays. Ordered arrays from bee honeycomb and several from the general field of nanoscience are compared. Accurate measures of the order in porous arrays are made using the discrete radial distribution function (RDF) and the Debye-Waller Factor (DWF) from 2-D discrete Fourier transforms calculated from the real-space data using MATLAB routines. Nanoporous anodized aluminum oxide, hexagonal arrays from functional materials, hexagonal arrays from nanosphere lithography, and arrays from block copolymer lithography (all taken from the literature) are compared to two-dimensional model systems. The DWF is normalized to the first harmonic and depends on N, the number of peaks in the fit for these finite arrays. We optimize N to the classical model for the DWF as a fit to reciprocal space K$^2$.

4:06PM W27.00009 Molecular Simulations of Liquid/Vapor Phase Equilibria for Single Component and Binary Mixtures of Nanoparticles, MARK HORSCH, PIETER INT VELD, JERMYE LECHMAN, GARY GREST, Sandia National Labs — Self-assembly of nano and colloidal particles into ordered structures is an important technological challenge for the design of future materials and devices. One promising self-assembly technique is the evaporation of nanoparticle suspensions in droplets. However, it is difficult to experimentally observe the self-assembly process in the evaporating droplet. Computer simulation provides an avenue with which to address and directly observe the self-assembly of model nano and colloidal particles within the droplet provided an efficient model can be developed. Here we present the liquid-vapor phase envelopes for model particles as a function of particle size. We compare the liquid/vapor phase envelopes and the computational efficiency for several different models including composite particles comprised of Lennard-Jones (LJ) atoms and particles interacting via integrated LJ potentials. Results for binary mixtures of nanoparticles in a solvent of LJ atoms will also be presented. These studies provide a framework for the size range of particles that can be addressed by each model. Sandia is a multiprogram laboratory operated by Sandia Corp., a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.
The search for molecular assemblies with interesting transport properties for molecular electronic devices is an active field of research. Isocyanide self-assembled monolayers (SAMs) have received some attention lately, as they may provide a better π-network for electron transport than other molecular SAMs such as benzenethiols. We have studied the structural and electronic properties of the interface between a gold surface and an aromatic isocyanide SAM, using density-functional theory in the GGA-PBE approximation. Our calculations predict a herringbone arrangement at high coverage, instead of the conventional structure with (√3 × √3)R30° periodicity. The most favorable geometry is however found at low coverage, where the interaction between molecules is negligible and the barriers between differently tilted geometries are small compared to room temperature. These results explain the disordered patterns recently observed in room temperature STM measurements and point at possible difficulties in using isocyanide SAMs for molecular devices. Our calculations also give insight into the alignment of the molecular energy levels with respect to the Fermi energy of the metal substrate, and the charge redistribution at the interface, which provide essential guidance for understanding and predicting transport properties of these SAMs, in case ordering can be achieved.

The electronic and structural properties of the self-assembled monolayer of Au-benzene-1,4-dithiol-Au molecules is essential to have a clear physical picture of the way these particles interact. To this end, we are investigating systems of metal nanoparticles ligated with alkyl chains. Our approach is three-fold. First, we are simulating (Monte Carlo) systems of ligated nanoparticles, including all chain/particle interactions in order to develop a model potential. Second, we are simulating (molecular dynamics) systems of these particles interacting via this model potential, varying the alkyl chain length, solvent, core material, and particle volume fraction. Finally, for comparison we are simulating these systems using theoretically derived potentials found in the literature. Initial results indicate a range of morphologies, from fractal aggregates to crystallites, depending on the temperature and potentials involved. Our goal is to provide a guide to researchers in choosing materials and assembly conditions that will lead to desired assembly properties.

Auger electron-hole scattering leads to efficient P → S electronic relaxation in self-assembled (In,Ga)As/GaAs quantum dots, which is within the range of known bond angles of S, e.g. 98.4° for SF5, 103° for SC12 and 96.4° for CH3(CH2)4SH. The Au 5d band is dominantly located at -2.3 eV below the Fermi level, E_F, with a sharp peak in the partial density of states (PDOS). The PDOS’s also show that the highest-occupied-molecular-orbital band contains S 3p, C 2p and Au 5d hybridized states, while the lowest-unoccupied-molecular-orbital band contains S 3p, C 2p and Au 5d hybridized states. The dominant Au 6s states are located at about -1.5eV and 1.3eV relative to E_F. The present result shows that Au 5d states, which are usually ignored in previous theoretical studies, play an important role in the S-Au bonding and contribute significantly to the transport property of the molecule.

This work was supported by the National Science Council of Taiwan. (Contract number: NSC 94-2112-M-110-012)

Supportied by DOE-SC-BES-DMS under NREL Contract DE-AC36-99GO10337

Thursday, March 8, 2007 2:30PM - 5:30PM
Session W28 DMP: Focus Session: Carbon Nanotubes: Transport and Thin Films
Colorado Convention Center 302

Hall Effect and Magnetoresistance of Single-walled Carbon Nanotubes S. H. JHANG, S. H. LEE, U. DETTLAFF, D. S. LEE, S. ROTH, Y. W. PARK, C. STRUNK, Institute of Experimental and Applied Physics, University of Regensburg — We report Hall coefficient and magnetoresistance measurements on films and networks of single-walled carbon nanotubes (SWNTs). Four different types of SWNTs are prepared as films; Purified SWNTs synthesized either by HiPCO (High-Pressure CO Conversion) process or by laser ablation method (laser SWNTs), and HiPCO and laser SWNTs chemically treated by SOCl2. SOCl2-modified SWNTs show higher conductivity due to doping effect. The measured Hall voltages are linear for all samples in fields up to 6 T. The carrier density of SWNTs is determined to be ~10^22 cm^-3 for HiPCO and ~10^21 cm^-3 for laser SWNTs. Considering that theoretically predicted carrier density of metallic SWNT is ~10^22 cm^-3 and that of semiconducting SWNT is ~10^21 cm^-3, the difference in carrier density between HiPCO and laser SWNTs can be originated from the difference in the ratio of metallic and semiconducting SWNTs in both films. While Hall coefficient is positive in the whole temperature range of 1.4 - 300 K for HiPCO and the Hall coefficient of laser SWNTs interestingly shows a sign change around at T = 15 K. The magnetoresistance of SWNTs studied in high magnetic fields up to 33 T, and in a temperature range of 0.4 - 300 K will be also presented.
Energy Anomaly and Polarizability of Carbon Nanotubes, DMITRY NOVIKOV, FTPI, University of Minnesota, and Princeton University. LEONID LEVITOV, Department of Physics, MIT — Electron properties of carbon nanotubes can change qualitatively by applying a strong perpendicular electric field. In metallic tubes the sign of Fermi velocity can be reversed by a sufficiently strong field, while in semiconducting tubes the effective mass can change sign. Changes in the spectrum manifest themselves in a breakup of the Fermi surface and in the energy gap suppression, respectively. The effect is controlled by the field inside the tube which is screened due to the polarization induced on the tube. The theory of screening is linked to the chiral anomaly for 1D fermions that reveals universality and scale invariance of the response dominated by π electrons. [Phys. Rev. Lett. 96, 036402 (2006)]

3:06PM W28.00004 Massive Integration of Nanotube/Nanowire-based Devices, SEUNCHUN HONG, Physics and Astronomy, Seoul National University — Although nanotube (NT)/nanowire (NW)-based devices are drawing an attention as next generation device architecture, a lack of massive assembly method has been holding back their practical applications. In this talk, we will present a massive integration strategy of NT/NW-based devices, where surface molecular patterns guide the ‘selective assembly’ and ‘alignment’ of various NTs/NWs (e.g. carbon NT, vanadium oxide NWs, etc) on virtually general substrates (e.g. Au, silicon oxide, Si, Al, etc). Interestingly, NT/NW adsorbed on solid substrates exhibit ‘2-dimensional sliding motions’ on the substrates to form desired device structures. This strategy is named here as ‘surface-programmed assembly’ in the sense that entire assembly process can be programmed by molecular patterns on the substrates to form molecular patterns. This process is utilized for wafer-scale fabrication of NT/NW-based devices such as high-performance transistors and bio-sensors. Importantly, since entire processing steps can be done by using only conventional microfabrication facilities without any high-temperature processing, the strategy is readily accessible for conventional device industry and may open up new ‘NT/NW-silicon hybrid device industry’ in the future. [REF: Nature 425, 26 (2003); Nature Nanotechnology 1, 66 (2006)]

3:42PM W28.00005 Quantum capacitance and gate coupling in NT array field effect devices, SLAVA V. ROTKIN, Lehigh University, JOHN A. ROGERS, Beckman Institute, UIUC — Modern electronics may essentially benefit on a new approach to fabricating nanotube field-effect thin film transistors (NT-TFT) that consist of parallel NT arrays with high uniformity of inter-tube spacing and orientation of neighbor N Ts. The large density of N Ts per channel area allows to improve device characteristics as drain current and transconductance. Here we address theoretically the issue of a quantum capacitance as a unique feature of the single-wall NT material and its role in transport in the dense or sparse array NT-TFTs. We present a complete electrostatic model joined with the quantum theory of the NT response to investigate the capacitance coupling to the backgate and/or the top gate for the broad range of the TFT device geometry. We vary the NT density, uniformity of the array, dielectric substrate and the top-gate dielectric to study the factors possibly limiting performance of the NT-array TFT. We found that due to the effect of strong electrostatic coupling between neighbor N Ts in the TFT channel the device characteristics, such as gate coupling and the conductance related to the latter, are robust even to significant deviations from an ideal geometry. This is discussed with respect to the problem of fabrication of devices with good uniformity at the system level despite of some disorder at the subsystem level of discrete elements. [Supported by NSF-0403489]

3:54PM W28.00006 Self-assembled Monolayers of Carbon Nanotubes and Their Properties, VLADIMIR SAMUJOV, JASELING KOO, Department of Materials Science, SUNYSB, JEAN CALIBERT, Laboratoire National des Champs Magnétiques Pulses, VITALY KSENEVICH, NIKOLAJ POKLONSKI, Department of Physics, State University of Belarus — Electronic and thermal transport properties of carbon nanotubes are of particular interest due to their potential use as components in nano electronics applications. Applications of the individual nanotubes are progressing rapidly. However, the electrical and thermal conductivity transport properties of the 2-D layers still fall short for the properties of the individual carbon nanotubes. We have developed a new method of self-assembling of carbon nanotubes (CNT) into high-density 2-D arrays without prior functionalization based on modified Langmuir-Blodgett technique. The method shows several major advantages over the conventional method of CNT monolayers formation. The electrical, thermal conductivity and magneto-transport properties of the monolayers (arrays) of multi-wall and single-wall carbon nanotubes in the temperature range 1.8-300K and in magnetic fields up to 35 T have been tested. Gas sensing properties of the self-assembled arrays of CNTs are discussed.

4:06PM W28.00007 Towards an optimal nanotube dispersion for transparent conductive coatings, MATTHEW GARRETT, University of Tennessee, ILIA IVANOV, BIN ZHAO, ALEX PURETZKY, DAVID GEOHEGAN, Oak Ridge National Laboratory — Thin films of carbon nanotubes have been investigated as a potential material for transparent conductive coatings. There is a range of transmission and resistance that must be met to make the film useful for technological applications, down to 101/Square at over 80%/T. When nanotubes in solution are made into thin films, the electro-optical properties of the film is dependent on the method of dispersion of the tubes used to make the film, in addition to the quality of the starting material used to make the dispersion. At 90%/T, the method of dispersion can cause nearly a factor of ten difference, 15000/ Square, in the resulting film’s resistance. Aggregates can cause scattering from the film, detracting from its transmission. The length and purity of the tubes affects the overall resistance of the film. The extent of tube bundling also plays an important role in the electro-optical properties of these films. Methods of quantifying the nature of tubes in solution can yield much insight into the quality of the film which will result from the solution. We have shown how a thorough characterization of the tubes during dispersion as well as after deposition is helpful in determining how to achieve the desirable attributes of a transparent conductive film of nanotubes.

4:18PM W28.00008 Ambient Formation of Aligned Carbon Nanotube Networks, MARCUS LAY, PORNNIPA VICHCHULADA, University of Georgia — Nano-scale electronic materials will play a roll of great significance in electronic devices of the near future. Carbon nanotubes (CNTs), in particular, show great technological promise. Yet, major obstacles to the incorporation of CNTs into practical electronic devices remain; one such challenge is the lack of a method to form ordered constructs of individual carbon nanotubes on a large scale. 2-dimensional networks of CNTs show potential as a method of circumventing the difficulties associated with lack of control over the physical and electrical properties of individual CNTs; for a random network of CNTs, transport properties in characteristics of individual CNTs become less important. Therefore, a 2-D network composed of a mixture of metallic and semiconducting CNTs behaves as a semiconductor above the percolation threshold for semiconducting nanotubes. A novel method of creating ordered arrays of purified CNTs has been developed to attain a higher level of control over reproducibility in CNT-based applications. This method uses unidirectional airflow to order CNTs in aqueous suspension and deposit them on a prepared surface. The result is an electrically continuous array of highly aligned CNTs. These ordered arrays of CNTs exhibit electrical conductivity over macroscopic lengths (up to 3’), and have shown promise in field-effect transistor (FET) applications.

4:30PM W28.00009 Geometry-dependent resistivity scaling in single-walled carbon nanotube films, ASHKAN BEHNAM, ANT URAL, Electrical and Computer Engineering, University of Florida — We study the resistivity scaling in transparent and conductive carbon nanotube films as a function of nanotube and device parameters. First, we observe experimentally that the nanotube film resistivity exhibits an inverse power law dependence on device width below a critical width of 2 microns. We then use Monte Carlo simulations to model this behavior and to study the effect of four parameters, namely tube-tube contact to nanotube resistance ratio, nanotube density, length, and alignment on resistivity and its scaling with device width. We observe stronger resistivity scaling with device width when the transport characteristics in the film are dominated by tube-tube contact resistance, or when the nanotube density, length, or alignment is increased. We also observe that, near the percolation threshold, the resistivity of the nanotube film exhibits an inverse power law dependence on all of these parameters, which is a distinct signature of percolating conduction. However, the strength of resistivity scaling for each parameter is different. We explain these observations, which are in agreement with experimental work, by simple physical and geometrical arguments. Nanoscale study of percolating transport mechanisms in nanotube films is essential for understanding and characterizing their performance in submicron devices.

Work sponsored by NSF-NIRT Grant DMR-0304019 and NSF MRSEC Grant No. DMR 02-13706.
4:42PM  W28.00010 Modeling of Nanotube Network Semiconductors. MEG NOAH, YOUNG-KYUN KWON, University of Massachusetts Lowell — Novel modeling techniques are used to characterize the structural, electronic and optical properties of nanocomposite network semiconductors. Ab initio computations of the structural properties of ensembles of nanotubes on a variety of substrates are presented. We use Monte Carlo and percolation simulations to predict manufacturing success rates given semiconductor design and processing constraints. The performance impact of flattening of nanotubes and topological defects on nanotubes will also be presented. The purpose of this study is to assist experimentalists and to stream-line and optimize nanomanufacturing. Our research focuses on the fundamental understanding of nanostructured materials and their application to molecular electronic devices.

1 Nanomanufacturing Center of Excellence and Center for High-rate Nanomanufacturing

4:54PM  W28.00011 Microwave Conductivity of Single Wall Carbon Nanotube Arrays. C. HIGHSTRETE, E.A. SHANER, MARK LEE, F.E. JONES, P.M. DENTINGER, A.A. TALIN, Sandia National Laboratories — We have measured the microwave conductivity spectra of carbon nanotube (CNT) parallel arrays from room temperature to 4K. Single wall CNTs were assembled by AC dielectrophoresis into parallel arrays of individual CNTs and ropes spanning the electrodes of coplanar waveguides (CPWs). The CPW complex reflection and transmission coefficients were measured from 0.1 to 50 GHz. Measurements of identical bare CPWs were utilized to calculate the frequency dependent complex conductivity and power dissipation of the CNT arrays and provide estimates of these quantities for individual CNTs in this configuration. Small loss due to the CNT arrays is consistently measured and increases with frequency.

5:06PM  W28.00012 Kohn anomalies and non-adiabaticity in doped carbon nanotubes. A. MARCO SAITTA, NICOLAS CAUDAL, MICHELE LAZZERI, FRANCESCO MAURI, IMPMC-Univ P et M Curie-Paris 6 — The tangential vibrational modes of metallic single-walled carbon nanotubes (SWNTs) are thought to be characterized by Kohn anomalies resulting from the combination of their intrinsic one-dimensional nature and a significant electron–phonon coupling. These properties are modified by the doping-induced tuning of the Fermi energy level $\epsilon_F$, obtained through the intercalation of SWNTs with alkali atoms or the application of a gate potential. We present a Density-Functional Theory (DFT) study of the vibrational properties of a (n,n) metallic SWNT as a function of electronic doping. For such study, we use, as in standard DFT calculations of vibrational properties, the Born-Oppenheimer (BO) approximation, but we also use time-dependent perturbation theory to explore non-adiabatic effects beyond this approximation. We compare our results with existing measurements and suggest features to be explored in future experiments.

5:18PM  W28.00013 Radiation Materials for Space Missions and Industries. RAM TRIPATHI, NASA Langley Research Center, Hampton, VA 23681 — NASA has a new vision for space exploration in the 21st Century encompassing a broad range of human and robotic missions including missions to Moon, Mars and beyond. Exposure from the hazards of severe space radiation in deep space long duration missions is "the show stopper." The great cost of added radiation shielding is a potential limiting factor in deep space missions. In the enabling technology, we have developed methodology and concomitant technology for optimized shield design over multi-segmented missions involving multiple work and living areas in the transport and duty phase of space missions. The total shield mass over all pieces of equipment and habitats is optimized subject to career dose and dose rate constraints. Studies have been made for various missions. Current technology is adequate for low earth orbit missions. Revolutionary materials need to be developed for career astronauts and deep space missions. The details of this new technology and its impact on space missions and other technologies will be discussed.

Thursday, March 8, 2007 2:30PM - 5:30PM – Session W29 DMP: Focus Session: Graphene V  Colorado Convention Center 303

2:30PM  W29.00001 Scanning tunneling microscopy of graphene field effect transistors. MASA ISHIHAGI, JIANHAO CHEN, ELLEN WILLIAMS, Physics Department and the Material Research Science and Engineering Center, University of Maryland, College Park, MD 20742 — We have investigated the electronic properties of graphene field effect transistors at atomic scale using scanning tunneling microscopy. We find that photoreis, required by conventional electron beam lithography, binds to graphene and leaves residues with thickness of approximately 1 nm. We will present the procedure necessary to eliminate this residue and report our results of scanning tunneling microscopy and spectroscopy performed on graphene.

1 This work is partially supported by the DCI postdoctoral fellowship and the Laboratory for Physical Sciences at University of Maryland.

2:42PM  W29.00002 Scanning Probe Microscopy studies of 2D and quasi-2D graphene crystal structures. ELENA POLYAKOVA, Columbia University, YUANBO ZHANG, University of California Berkeley, MELINDA HAN, PHILIP KIM, GEORGE FLYNN, Columbia University, COLUMBIA UNIVERSITY, NSEC COLLABORATION, COLUMBIA UNIVERSITY, CHEMISTRY COLLABORATION — In these studies we utilize a variety of Scanning Probe techniques to observe evolution of material properties as a result of transitions from 3D to 2D crystal structures. Graphite is an ideal candidate for these studies as it stands alone 2D crystal (graphene) and quasi-2D films are conductive, stable, and chemically inert under ambient conditions. These crystals can be easily deposited on an oxidized silicon wafer, and the number of atomic layers can be precisely counted. Specific examples will be given to relate local and mesoscopic properties of these crystals as a function of the number of graphene monolayers forming the crystal. The role of the interaction between the substrate and graphene films will be considered. The finite thickness of crystals allows us to examine defects formed not only on the surface of the film but also below the topmost layer. Attenuation of corrugation in Scanning Tunneling images by overlays of graphene is described. Compatibility of graphene films with atomic-scale electronics will be discussed.

2:54PM  W29.00003 Imaging Electronic Interference Effects in Ultrathin Epitaxial Graphite. JASON CRAIN, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899-8412, USA, GREGORY RUTTER, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899-8412, USA, TIANBO LI, PHILLIP FIRST, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 — We have used scanning tunneling microscopy and spectroscopy at 4K to investigate local fluctuations in the electronic structure of ultrathin epitaxial graphite grown on SiC. Spectroscopic maps of the density of states for two- and three-layer films reveal spatial modulations that fluctuate with energy. These maps show short range root three by root three ordering reminiscent of Bloch wave interference observed in finite carbon nanotube segments [1]. Additional long range fluctuations have a characteristic length scale that may be related to the underlying structure of the SiC interface.


3 This work is supported in part by the Office of Naval Research and NSF.
We discuss the resulting electronic structure and possible consequences for transport properties. [1] Z. Rong and P Kuiper, Phys. Rev B. 48, 17427, (1993) at low energies (close to the Dirac points of the uncoupled bilayers) and for small rotation angles, based on a continuum approximation for the uncoupled layers.

resulting from a small angle rotation of the top layer have been observed in graphite [1]. We consider a similar situation in a graphene bilayer. We determine

\[ \pi \] momentum. However, they hardly depend on the direction of the transferred momentum and the temperature. There are three low-frequency plasmon modes in the AA- and AB-stacked plasmons exhibit the similar \( \pi \) plasmons. The first low-frequency plasmon behaves as a acoustic plasmon, and the others belong to optical plasmons. Bilayer graphene quite differ from the monolayer graphene and the AB-stacked bulk graphite, such as the low-frequency plasmons and the small-momentum \( \pi \) plasmons.

3:42PM W29.00007 Correlation Energy of Graphene . VALERI KOTOV, A. H. CASTRO NETO, Boston University — We discuss the ground state energy of an electron gas on a honeycomb lattice (graphene), where the quasiparticle spectrum has Dirac structure, i.e. linear energy-momentum relation. The correlation energy, due to electron-electron interactions, is calculated in the two-loop approximation, which is the first correction to the Hartree-Fock energy. The possibility of inhomogeneous states is discussed.

3:54PM W29.00008 Electromechanical instabilities of suspended carbon nanotubes - multi mode excitations , MAGNUS JONSSON, LEONID GORELIK, Department of Applied Physics, Chalmers University of Technology, SE-412 96 Gothenburg, ROBERT SHEKHTER, MATS JONSON, Department of Physics, Goteborg University, SE-412 96 Gothenburg — We have theoretically investigated electromechanical instabilities of suspended carbon nanotubes when using an STM-tip to probe the suspended part of the tube. A coupling between the vibrational modes of the nanotube and tunneling electrons may lead to a pumping of energy into the mechanical subsystem, resulting in large amplitude vibrations of the CNT. This effect is related to the “shuttle instability” and changes the transport properties of the system. In the present study, instability of different bending modes have been investigated. We show that, with respect to the instability, different modes can be treated independently in the limit of weak electromechanical coupling. Also, we show that excitations of different modes are controlled by the vibration frequency and tunneling rates. Tuning rates of the order of the frequency are found optimal for an instability to occur. Hence, a selective excitation of a single mode is possible. We analyze the limit cycle behavior in this case. Another scenario is simultaneous excitation of several modes, leading to a complex behavior in stationary regime.

4:06PM W29.00009 Electronic properties of graphene multilayers , FRANCISCO GUINEA, Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco. 28049 Madrid. Spain., ANTONIO H. CASTRO NETO, Department of Physics. Boston University. 590 Commonwealth Av. Boston MA02115, NUNO M.R. PERES, Departamento de Física. Universidade do Minho. Braga. P-4710-057 Portugal — The electronic structure, screening properties, and charge distribution in stacks of graphene layers is studied. We analyze: i) The stability of Dirac points as function of the ordering of the stack and the number of layers, ii) The existence of surface bands at the top and bottom layers for some stack orderings, iii) The appearance of gaps induced by inhomogeneous charge distributions, and iv) The charge induced by external electric fields. We find that electronic bands with linear, Dirac like, dispersion exist in stacks with the Bernal stacking and an odd number of layers, and for rhombohedral stacking. In the last case, a dispersionless surface band is also formed. In the presence of interlayer hopping, the dielectric response of a stack with the Bernal ordering favors the formation of a charge density wave with periodicity equal to twice the interlayer spacing. In doped stacks, the charge will accumulate at the surfaces, and present an even-odd modulation.

4:18PM W29.00010 Local density of states of graphene with diagonal and off-diagonal disorder , N.M.R. PERES, JOAO RICARDO SANTOS, School of Sciences, Physics Department, F. KLIRONOMOS, SHAN-WEN TSAI, University of California, Riverside, Physics Department, J.M.B. LOPES DOS SANTOS, University of Porto, Physics Department, A.H. CASTRO NETO, Boston University, Physics Department — We study the effect of diagonal and off-diagonal disorder in the local density of states of a graphene sheet. The exact Green’s functions for graphene in the presence of a local potential and in the presence of a modification of the local hopping parameter are given. A discussion of the resonances induced by disorder in the local density of states is provided. We obtain the exact Green’s function for a vacancy as a limiting procedure applied to the Green’s functions with either diagonal or off-diagonal disorder. The exact Green’s function in the presence of both local and off-diagonal disorder is given.

4:30PM W29.00011 Moire patterns in graphene bilayers: electronic structure1. JOAO LOPES DOS SANTOS, CFP, Dep Fisica, Faculdade Ciencias, Universidade do Porto, NUNO PERES, Departamento Fisica, Universidade do Minho, ANTONIO CASTRO NETO, Department of Physics, Boston University, EDUARDO CASTRO, CFP, Dep. Fisica, Faculdade Ciencias, Universidade do Porto — Moire patterns, resulting from a small angle rotation of the top layer have been observed in graphite [1]. We consider a similar situation in a graphene bilayer. We determine the angles for which the resulting structure is periodic and study its symmetries. We develop a general formalism for the calculation of the electronic properties at low energies (close to the Dirac points of the uncoupled bilayers) and for small rotation angles, based on a continuum approximation for the uncoupled layers. We discuss the resulting electronic structure and possible consequences for transport properties. [1] Z. Rong and P Kuiper, Phys. Rev B. 48, 17427, (1993)

1Support from EU and FCT, Portugal, is acknowledged.
4:42PM W29.00012 Experimental signatures of topological defects in graphene. ANDREW IYENGAR, HERBERT FERTIG, Indiana University, LUIS BREY, Instituto de Ciencia de Materiales de Madrid — We study the electronic structure of graphene with topological defects, in which some of the hexagonal plaquettes of the honeycomb lattice are replaced by pentagons or heptagons. Our tight-binding calculations show that the local electronic density of states becomes particle-hole asymmetric in the vicinity of such defects. This provides a means of experimentally distinguishing so-called “plastic” curvature from elastic deformation. We evaluate various analytic approaches to these defects and discuss their effects on scattering and transport.

4:54PM W29.00013 Direct Observation of Interface States between Single Layer Graphene and SiC*. GREGORY RUTTER, TIANBO LI, PHILLIP FIRST, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, JASON CRAIN, EMILY JARVIS, NATHAN GUSINGER, MARK STILES, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899 — Graphite films grown on carbon-terminated SiC exhibit coherent transport properties that suggest potential for novel nanoelectronics applications [1]. However, for films grown on silicon-terminated SiC the spin-orbit interaction is greatly reduced, so that the interface electronic structure influences the transport [1]. We have investigated the interface structure and electronic states that form in single layer graphene grown on silicon terminated SiC, using scanning tunneling microscopy and spectroscopy measurements at 4 K. Imaging a single graphene layer reveals features of both the graphite structure and the SiC interface. Which structure dominates is observed to be a function of the imaging bias. Sharp peaks in the density of states were found over SiC interface features, which correlate to the onset voltages observed in topography measurements. A comparison of experimental and theoretical findings will be discussed including relevance to transport measurements. *This work is supported in part by the Office of Naval Research and NSF. [1] C. Berger et al., Science 312, 1191 (2006); J. Phys. Chem. B 108, 19912 (2004).

5:06PM W29.00014 Graphene-based Silica Composite Thin Films. SUPINDA WATCHAROTONE, DMITRY DIKIN, SASHA STANKOVICH, RICHARD PINER, GEOFFREY DOMMETT, INHWA JUNG, GUENNADI EVMENENKO, RODNEY RUOFF, Northwestern University, Evanston, Illinois, SHANG-EN WU, SHU-FANG CHEN, CHUAN-PU LIU, National Cheng Kung University, Tainan, Taiwan — Very thin, smooth, transparent, and electrically conductive silica films with embedded graphene-based sheets were fabricated via the sol-gel route. Individual ‘graphene oxide’ sheets exfoliated in water were incorporated into silica gels. Composite films were formed by spin coating and rendered conductive by treatment with hydrazine, followed by curing at 400 °C under nitrogen flow. The films were studied by SEM, AFM, TEM, X-ray reflectivity, XPS, UV-Vis spectroscopy, and the electrical conductivity was measured. Transparent and conductive thin silica composite films approximately 30 nm thick were fabricated on glass and silicon substrates, opening up new possibilities for making glassy materials with moderate conductivity and high optical transparency. Support from NASA (NCC-1-02037) through the University Research, Engineering and Technology Institute on Bio-inspired Materials and the NSF (CMS-0510212) is appreciated.

5:18PM W29.00015 Preparation and transport studies of single layer graphite oxide and graphene films. SONG HAN, Electrical Engineering Department, University of California, Los Angeles, SCOTT GILJE, RICHARD KANER, Department of Chemistry and Biochemistry, University of California, Los Angeles, KANG WANG, Electrical Engineering Department, University of California, Los Angeles — Single sheet graphite oxide films are synthesized by intercalation and exfoliation routes of graphite. Because of its layered structure, graphite can readily be intercalated using alkali metals. Such method opens up the possibility of synthesizing ultra-thin layers of graphite by reducing the graphite oxide films. The as-synthesized graphite oxide films are deposited on SiO2/Si substrates. Ebeam lithography is used to fabricate graphite oxide Field Effect Transistors (FETs). The transport properties of these devices are studied before and after the reduction of graphite oxide films.

Thursday, March 8, 2007 2:30PM - 5:30PM – Session W44 DMP: Focus Session: Nanoscale Transport - Mostly Quantum Dots Colorado Convention Center 507

2:30PM W44.00001 Spin-Lattice Relaxation Rate in Lateral Quantum Dots. SAMI AMASHA, Massachusetts Institute of Technology — Laterally gated quantum dots (QDs) fabricated on AlGaAs/GaAs heterostructures show promise for spin-based quantum computation. One limit to the coherence time in QDs, which sets the timescale on which quantum operations must be completed, comes from the spin-orbit interaction. In a magnetic field \( B \) the spin states of a single electron in a QD are split by the Zeeman energy \( g_\mu_B B \); the spin-orbit interaction couples the spin states of a QD to its orbital degrees of freedom, which in turn can interact with piezoelectric phonons to relax the spin from the excited state to the ground spin state. The time scale over which this happens is the relaxation time \( T_1 \). We present measurements of the relaxation rate \( 1/T_1 \) of one electron in a single laterally gated QD at magnetic fields down to 1 T, much lower than previously measured. These measurements are possible because of the good quality of the AlGaAs/GaAs heterostructure we have used combined with an active feedback system that compensates for residual drift and switches of the dot energy levels. We find that \( T_1 \) is as long as 1 s at 1 T. We compare our measurements to theoretical predictions of \( T_1 \) caused by spin-orbit coupling to phonons and extract the spin-orbit length, which describes the strength of the spin-orbit interaction. This demonstrates that spin-orbit coupling to phonons can account for the observed long relaxation times.

3:06PM W44.00002 Spin Blockade in electronic transport through quantum dots. BHASKARAN MURALIDHARAN, SUPRIYO DATTA, Purdue University — Recently, Spin Blockade (SB) transport through quantum-dots has attracted attention owing to potential applications in quantum state control. In this talk, we identify the mechanism underlying current collapse (NDR), current leakage and bias dependent asymmetry in the I-V characteristics of quantum dot systems, which characterize spin blockade transport. As a specific example of this generic mechanism, we examine the conditions for SB to occur in transport through coupled quantum dots. This leads to a consistent interpretation of the non-trivial features in the experimental I-Vs of coupled quantum dots including multiple NDR, gate-able current collapse, and current rectification. Most importantly, our study elaborates on how a delicate interplay of orbital energy offset, delocalization, and Coulomb interaction between conduction electrons localized on either dot, strongly influences the aforementioned transport signatures.

3:18PM W44.00003 Resonant dephasing of the electronic Mach-Zehnder interferometer. EUGENE SUKHORUKOV, University of Geneva, VADIM CHEIANOV, Lancaster University — We address the recently observed unexpected behavior of Aharonov-Bohm oscillations in the electronic Mach-Zehnder interferometer experimentally realized in a quantum Hall system [1]. We argue that the measured lobe-like structure in the visibility of oscillations and the phase rigidity result from a long-range local interaction between two adjacent counter-propagating edge states, which leads to a resonant scattering of bosonic charge excitations. The visibility and phase shift, expressed in terms of the transmission coefficient for bosons, provide the tool for investigating the nature of quantum Hall edge states. [1] I. Neder et al., Phys. Rev. Lett. 96, 016804 (2006).

*The work is supported by the Swiss NSF.
3:30PM W44.00004 Electron population control of an isolated quantum dot using surface-acoustic-wave pulses. CHRIS FORD, ROBERT SCHNABLE, MASAYA KATAOKA, ADAM THORN, CRISPIN BARNES, DAVID ANDERSON, GEB JONES, IAN FARRER, DAVID RITCHIE, MICHAEL PEPPER, University of Cambridge — In developing quantum information technology, isolation from the environment is a key for long coherence times. However, many quantum-dot (QD) experiments require a fair degree of coupling to electron reservoirs. The electron number becomes progressively difficult to control as the degree of isolation increases and the electron dwell time exceeds the timescale of experiments. In such a system, a means to transfer electrons on demand between a QD and another QD or reservoir is desirable. We report our recent experiments on sending surface acoustic waves (SAWs) past a QD that is isolated from the leads by strong barriers, such that electrons take hundreds of seconds to tunnel. A short pulse of SAWs is used to characterize the electronic structure of the QD, and to transport electrons in and out of the QD. The mechanism of electron transfer from dynamic QDs defined by the SAWs themselves into a gate-defined static QD is investigated. This has applications for quantum information transfer and processing.

3:42PM W44.00005 Coulomb-energy-dependent tunnelling from few-electron dynamic quantum dots defined by surface acoustic waves. MICHAEL ASTLEY, MASAYA KATAOKA, CHRIS FORD, CRISPIN BARNES, DAVID ANDERSON, GEB JONES, IAN FARRER, DAVID RITCHIE, MIKE PEPPER, Cavendish Laboratory, University of Cambridge — Electrons confined in dynamic quantum dots (DQDs) have been proposed as an implementation for the control and manipulation of quantum information. In this scheme, entanglement is achieved at a tunnel barrier between neighbouring DQDs. In this presentation we investigate the escape rate from a DQD at a tunnel barrier. One or few electron DQDs were created by a surface acoustic wave travelling through a pinched-off channel, isolated from a reservoir by a narrow tunnel barrier. The tunnelling rates across the barrier were determined using a rate-equation model, and found to increase with the electron occupation of the DQD. This effect can be explained in terms of Coulomb interactions between the confined electrons.

3:54PM W44.00006 Conductance signatures of a quantum-critical transition and a Kondo filtered resonance in double quantum dots1. LUI S DIAS, NANCY SANDLER, Ohio University, KEVIN INGERSENT, University of Florida, SERGIO ULLOA, Ohio University — We present conductance results for double quantum dot (DQD) systems containing one dot in the Kondo regime coupled to an effectively noninteracting dot. The system is mapped onto a single impurity Anderson model with a structured (nonconstant) density of states [1]. The linear conductance is obtained using the DQD’s Green’s function calculated from numerical renormalization-group calculations for both side-dot and parallel configurations. In the side dot case, the conductance shows signatures of the band filtering through the resonant dot. This mechanism can be interpreted as an interference between many-body and single-particle states, splitting the Kondo resonance while preserving the Kondo singlet ground-state. In the parallel configuration, interference between conducting channels through the dots create a pseudogapped effective density of states [1]. We discuss possible approaches for detecting the quantum-critical point separating Kondo and non-Kondo phases in conductance measurements. [1] L.G.G.V. Dias da Silva et al, PRL 97 096603 (2006)

1Supported by NSF DMR 0312939, NSF-IMC and NSF-NIRT grants.

4:06PM W44.00007 Kondo effect in a quantum dot via orbital population switching1. HYUN-WOO LEE, Pohang University of Science and Technology, SEJOONG KIM, Massachusetts Institute of Technology — Strong correlation effects in electron transport through a spinless quantum dot are considered. For general tunneling matrix elements between the quantum dot and leads, there exists a conserved pseudospin degree of freedom when two orbitals in the quantum dot are degenerate. The fluctuations of the pseudospin at the quantum dot give rise to the Kondo effect described by the anisotropic $t$-$J$ model. Interestingly the Kondo effect generates a pair of asymmetric conductance peaks near the center of a Coulomb valley, in clear contrast to the conductance behavior due to the spin Kondo effect. This explains the origin of the so-called correlation-induced resonances reported recently [V. Meden and F. Marquardt, Phys. Rev. Lett. 96, 146801 (2006]). An exact relation to the phenomenon of the population switching is provided and differences from the conventional Kondo effects are clarified.

1This work was supported by the SRC program and the Basic Research Program of MOST/KOSEF.

4:18PM W44.00008 Modeling of tunneling spectroscopy of a single quantum dot involving two levels . MING TING KUO, National Central University, YIA-CHUNG CHANG, Academia Sinica — We have employed the two-level Anderson model to simulate the system of the tip/quantum dot (QD)/substrate double barrier junction. The tunneling current through the ground state and the first excited state in the cases of shell-tunneling and shell-filling is theoretically investigated in the framework of nonequilibrium Green’s function technique by solving the two level Anderson model properly. We found that single-particle and two-particle occupation numbers significantly influence the probabilities of each resonant energies arising from the intralevel and interlevel Coulomb interactions. Compared with tunneling current spectra of CdSe QDs, we predict some resonant structures which can be observed in an isolated QD.

4:30PM W44.00009 Band filtering and quantum phase transition in an asymmetric double quantum dot1. W. BRIAN LANE, K. INGERSENT, U. of Florida, L. G. G. V. DIAS DA SILVA, N. P. SANDLER, S. E. ULLOA, Ohio U. — Double quantum dots (DQDs) are currently of great theoretical and experimental interest. A DQD device in which one of the dots is in the Kondo regime and the other is effectively a noninteracting resonant level has been shown [1] to reduce to an effective one-impurity Anderson problem with a structured (nonconstant) density of states. Depending on QD parameters that can be controlled experimentally via gate voltages, such a device can exhibit zero-field splitting of the Kondo resonance on the interacting dot, or it can be tuned to access a quantum critical point separating Kondo-screened and local-moment phases. Using numerical renormalization-group techniques, we explore the robustness of these phenomena by increasing the Coulomb interaction on the resonant dot away from zero. We report the effects of the interaction on the device’s magnetic susceptibility, spectral function, and linear conductance. [1] L. G. G. V. Dias da Silva, N. P. Sandler, K. Ingersent, and S. E. Ulloa, Phys. Rev. Lett. 97, 096603 (2006).

1Supported by NSF Grants DMR-0312939 and DMR-0304314.

4:42PM W44.00010 Imaging Electron Flow From a Quantum Point Contact. M. P. JURA, M. A. TOPINKA, A. R. SCIambi, D. GOLDHABER-GORDON, Stanford University, L. URBAN, University of Illinois at Urbana-Champaign, A. YAZDANI, Princeton University, H. SHTRIMAN, Weizmann Institute of Science, L. N. PFEIFFER, K. W. WEST, Bell Labs, Lucent Technologies — We image electron flow from a quantum point contact (QPC) into a high-mobility two-dimensional electron gas (2DEG) using scanning gate microscopy (SGM). We note two surprising phenomena, which we compare with results from simulations: 1. The beam of electrons immediately leaving the QPC is unexpectedly narrow and collimated. 2. Under certain conditions, the signal generally associated with current flow density (i.e. the change in differential conductance due to scattering from the scanning gate tip) can change sign from negative to positive.
The theory predicts that the Kerr angle is proportional to the square of the superconducting energy gap and is inversely proportional to the cube of frequency, $\propto \frac{\Delta^2}{\omega^3}$. For Sr$_2$RuO$_4$, the polar Kerr angle agrees by the order of magnitude with the recent experimental measurement in [1].

$\frac{x}{y}$

In order not to heat up the sample locally at such low temperatures, we have observed non-zero Kerr rotations as big as 65 nanorad appearing below $T_c$. Our results imply a broken time reversal symmetry state in the superconducting state of Sr$_2$RuO$_4$, similar to $^3$He-A. More recent results on other oxide superconductors will also be described. This work was supported by Center for Probing the Nanoscale, NSF NSEC Grant 0425897 and by the Department of Energy grant DEFG03-01ER45925.

1. Performed in collaboration with B. K. Foster, R. G. Harris, L. S. Mattos, and G. Zeltzer. Work supported by the NSF, ONR, DOE, and the NDSEG Fellowship Program.

Friday, March 9, 2007 8:00AM - 11:00AM —
Session X8 DMP: Focus Session: Novel Superconductors VII: Triplet Pairing and Time Reversal Symmetry Breaking
Colorado Convention Center Korbel 1C

8:00AM X8.00001 High Resolution Polar Kerr Effect Measurements of Sr$_2$RuO$_4$: Evidence for Broken Time Reversal Symmetry in the Superconducting State$^1$. JING XIA, Department of Physics, Stanford University, Stanford, CA 94305 — Strontium ruthenate (Sr$_2$RuO$_4$) is an odd-parity superconductor, which has odd orbital angular momentum and symmetric spin-triplet (p-wave) pairing. Some of the possible p-wave states can further break time-reversal symmetry (TRS), since the condensate has an overall magnetic moment because of either the spin or orbital (or both) parts of the pair wave function. However, this TRS-breaking moment will be screened by the Meissner effect. Previously, tests for broken time-reversal symmetry in Sr$_2$RuO$_4$ relied on surfaces and defects where the Meissner screening is not perfect. However, for an unabating determination of the magnetic moment, a bulk measurement, such as measuring magneto-optic like effects, on high quality crystals, is needed. To this end we developed a new technique of measuring Polar Kerr Effect (PKE) at temperatures much below the transition temperature of Sr$_2$RuO$_4$ of 1.5 K. The technique is based on a fiber Sagnac interferometer with a zero-area Sagnac loop. This new technique allowed us to measure PKE with an accuracy of 10 nano-radian at 400 mK, while rejecting other artifacts like linear birefringence of the sample. The incident optical power was set to be below 2 micro-Watts in order not to heat up the sample locally at such low temperatures. We have observed non-zero Kerr rotations as big as 65 nanorad appearing below $T_c$. Our results imply a broken time reversal symmetry state in the superconducting state of Sr$_2$RuO$_4$, similar to $^3$He-A. More recent results on other oxide superconductors will also be described. This work was supported by Center for Probing the Nanoscale, NSF NSEC Grant 0425897 and by the Department of Energy grant DEFG03-01ER45925.

$^1$ Collaborators: Yoshiteru Maeno, Peter T. Beyersdorf, M. M. Fejer, E. Schlemm and Aharon Kapitulnik

8:36AM X8.00002 Theory of the high-frequency chiral optical response in a $p_x + ip_y$ superconductor$^1$. VICTOR YAKOVENKO, University of Maryland — The optical Hall conductivity and the polar Kerr angle are calculated as functions of temperature for a two-dimensional chiral $p_x + ip_y$ superconductor, where the time-reversal symmetry is spontaneously broken. The theoretical estimate for the polar Kerr angle agrees by the order of magnitude with the recent experimental measurement in Sr$_2$RuO$_4$ by XIA et al., Phys. Rev. Lett. 97, 167002 (2006). The theory predicts that the Kerr angle is proportional to the square of the superconducting energy gap and is inversely proportional to the cube of frequency, which can be verified experimentally. Reference: cond-mat/0608148.

8:48AM X8.00003 Instability of Singlet Superconductivity with Respect to the Appearance of a Triplet Component in a Vortex Phase.$^1$. ANDREI LEBED, OMJYOTI DUTTA, Dept. of Physics, University of Arizona — We show [1] that a vortex phase in a singlet d(s)-wave superconductor is absolutely unstable with respect to a generation of a triplet component of a superconducting order parameter. The triplet component, which appears for both attractive and repulsive interactions in a triplet channel, is shown to break three important symmetries of an internal superconducting order parameter: spin-rotational, parity [1], and time-reversal [2] ones. As a result, Cooper pairs are characterized by non-zero angular momenta [2] and non-zero spins [1], polarized in a plane, perpendicular to the external magnetic field. The above mentioned effects are expected to be of the order of unity in almost all modern superconductors such as MgB$_2$, high-Tc, organic, and some others. [1] A.G. Lebed, Phys. Rev. Lett. 96, 037002 (2006). [2] Omjyoti Dutta and A.G. Lebed, Nature, submitted (2006).
interferometer with a zero-area Sagnac loop. With this technique we show a shot-noise-limited sensitivity of 100 nanorad/doping levels. In order to be able to measure effects beyond our old search for anyon superconductivity, we devised a new technique based on a fiber Sagnac interferometry measurements. By using a non-equilibrium green function formalism, we find exact analytic expressions for the tunneling current and noise and identify experimental signatures of the Majorana nature of the bound states to be found in the shot noise. We discuss the results in the context of different candidate materials that are believed to support triplet superconductivity.

Superconductors: Evidence for Broken Time Reversal Symmetry Below the Pseudogap

Belitz, University of Oregon — In wave superconductors, topological excitations known as skyrmions are allowed, in addition to the usual vortices. In strongly type-II materials in an external magnetic field, a skyrmion flux lattice is expected to be energetically favored compared to a vortex flux lattice. We analytically calculate the energy, magnetization curves, and elasticity of skyrmion flux lattices in wave superconductors near the lower critical field and use these results with the Lindemann criterion to predict their melting curve. In striking contrast to vortex flux lattices, which always melt at an external field greater than the critical field, skyrmion flux lattices never melt near the critical field. This provides a simple and unambiguous test for the presence of skyrmions. In addition, the internal magnetic field distributions (which are measurable by muon spin rotation techniques) of skyrmion and vortex lattices are very different.

Skyrmion Flux Lattices in wave Superconductors

Skyrmion Flux Lattices in wave Superconductors

Work supported by the Department of Energy DE-AC02-76SF00515

9:00AM X8.00004 Broken time-reversal symmetry in a vortex phase of a superconductor under perpendicular magnetic field. OMIJOTI DUTTA, ANDREI LEBED, Dept. of Physics, University of Arizona — A vortex phase in a singlet superconductor is absolutely unstable with respect to a generation of a triplet component of a superconducting order parameter. The triplet component, which appears for both attractive and repulsive interactions in a triplet channel, breaks spin-rotational and parity symmetries.[1] Here we show[2] that in a perpendicular magnetic field, in addition to the above mentioned symmetries, the order parameter also breaks time reversal symmetry. As a result, Cooper pairs carry non-zero angular momenta. The above mentioned effects are expected to be of the order of unity in almost all modern superconductors such as high-Tc and organic ones. We suggest experimental studies to discover triplet-singlet mixing phenomenon which characterizes this novel type-IV superconductivity. [1] A. G. Lebed, Phys. Rev. Lett. 96, 037002. [2] O. Dutta and A. G. Lebed, Nature, submitted (2006)

9:12AM X8.00005 Aligning chiral order parameter domains in Sr2RuO4: Josephson interferometry measurements. FRANCOISE KIDWINGIRA, J.D. STRAND, D.J. VAN HARLINGEN, University of Illinois at Urbana-Champaign, Y. MAENO, Kyoto University — There is compelling evidence that the ruthenate superconductor Sr2RuO4 forms chiral order parameters of the form px+i.py and px-ipy. In zero magnetic field, these states are degenerate and result in the formation of a dynamical domain structure that has been detected by Josephson interferometry experiments. However, the degeneracy between the order parameters can be lifted by applying a magnetic field while cooling the system through the superconducting transition. We present Josephson interferometry measurements on field-cooled Josephson junctions that show evidence for domain alignment, manifested by the enhancement of the critical current and qualitative changes of the critical current modulation pattern in applied magnetic field. We also report evidence for memory effects in the domain chirality. [1] Francoise Kidwingira et al., Science, October 26 2006 (10.1126/science.1133239).

9:24AM X8.00006 Probing Bound States in p-wave Superconductors using Shot Noise. C.J. BOLEICH, Rice University, EUGENE DEMLER, Harvard University — The zero-energy bound states at the edges or vortex cores of chiral p-wave superconductors are expected to behave like Majorana fermions. We introduce a model Hamiltonian that describes the tunneling process when electrons are injected into such states. Using a non-equilibrium green function formalism, we find exact analytic expressions for the tunneling current and noise and identify experimental signatures of the Majorana nature of the bound states to be found in the shot noise. We will discuss possible origins of this effect in the context of different candidate materials that are believed to support triplet superconductivity.

9:36AM X8.00007 Skyrmion Flux Lattices in p-wave Superconductors.

9:48AM X8.00008 Probing the superconducting order parameter of UPt3 by Josephson Interferometry. J.D. STRAND, F. KIDWINGIRA, D.J. VAN HARLINGEN, University of Illinois at Urbana-Champaign, J.P. DAVIS, W.P. HALPERIN, Northwestern University — The unconventional superconductor UPt3 exhibits two superconducting transitions which are believed to correspond to two distinct superconducting phases. The symmetry of the order parameter in these phases has yet to be determined and the origin of the double transition remains an open question. We have fabricated Josephson junctions by evaporating copper and lead films onto UPt3 single crystals. Using a SQUID potentiometer, we observe critical currents that onset at the upper transition temperature of the crystal and use these results with the Lindemann criterion to predict their melting curve. In striking contrast to vortex flux lattices, which always melt at an external field greater than the critical field, skyrmion flux lattices never melt near the critical field. This provides a simple and unambiguous test for the presence of skyrmions. In addition, the internal magnetic field distributions (which are measurable by muon spin rotation techniques) of skyrmion and vortex lattices are very different.

9:00AM X8.00009 High Resolution Polar Kerr Effect Measurements of High-Temperature Superconductors: Evidence for Broken Time Reversal Symmetry Below the Pseudogap

10:00AM X8.00009 High Resolution Polar Kerr Effect Measurements of High-Temperature Superconductors: Evidence for Broken Time Reversal Symmetry Below the Pseudogap

This work was supported by Center for Probing the Nanoscale, NSF NSEC Grant 0425897 and by the Department of Energy grant DEFG03-01ER45925.

10:12AM X8.00010 Scanning magnetic imaging of strontium ruthenate (Sr3RuO4). CLIFFORD HICKS, Department of Applied Physics, Stanford University, YOSHITERU MAENO, Department of Physics, Kyoto University, KATHRYN MOLER, Department of Applied Physics, Stanford University — Strontium ruthenate is a spin-triplet superconductor with very likely, a time-reversal symmetry breaking px±ipy orbital order parameter. This is suggested by several experiments, including recent observation of a Kerr effect that develops when Sr2RuO4 becomes superconducting. Such an order parameter should result in spontaneous edge and domain wall currents which would generate a real-space magnetic signal, but this field yet to be observed. Currently it is estimated that, within the sample and near an edge (in the bulk it is Meissner screened), the field should peak at about 6G. We believe the spontaneous field may not be significantly smaller. We discuss its observability through scanning magnetic probe microscopy and describe current experimental efforts to image and measure this field.

[1] This work was supported by Center for Probing the Nanoscale, NSF NSEC Grant 0425897 and by the Department of Energy grant DEFG03-01ER45925.

[1] Work supported by the Department of Energy DE-AC02-76SF00515.
10:24AM X8.00011 Photoemission study of doping in the strontium ruthenate family , TIM KIDD.
University of Northern Iowa, TONICA VALLA, JOHN RAMEAU, PETER JOHNSON, Brookhaven National Laboratory — How dopants are incorporated into low dimensional correlated electron systems and their effects on such materials remain open questions despite an intense research effort over the past few decades. We have used photoemission spectroscopy to investigate the effects of dopants in these systems to measure their influence on electronic properties and phase transitions. In systems such as the high-Tc superconductors, disorder in the spatial distribution of dopants leads directly to nanoscale electronic disorder in the system. Despite this seeming randomness, photoemission studies have shown the electronic states become more well-defined with increasing concentration of dopants. In these systems, however, the dopants are usually incorporated outside the copper oxygen planes important for conduction and superconductivity. Here, we present photoemission data from the strontium ruthenate family that incorporate dopants directly into the conducting planes. Our results indicate that even relatively high dopant concentrations do not necessarily cause a large degree of disorder based broadening in the spectra. We have also detailed the influence of dopants like titanium on the associated magnetic and superconducting phase transitions in these materials.

10:36AM X8.00012 Mixed pairing state in Ru microdomains embedded in bulk single-crystal Sr$_2$RuO$_4$. ZHENYI LONG, KELLY MCCARTHY, CHRYSAFIS ANDREOU, DAVID CA Ven. The Pennsylvania State University, ZHIQIANG MAO, Tulane University, HIROSHI YAGUCHI, YOSHITERU MAENO, Kyoto University, YING LIU, The Pennsylvania State University — We performed detailed tunneling measurements on Ru microdomains embedded in Sr$_2$RuO$_4$ using In-Ru/Sr$_2$RuO$_4$ junctions prepared by pressuring freshly cut pure In wire onto a cleaved ab face of a Ru-containing Sr$_2$RuO$_4$ single crystal. We observed a superconducting transition temperature of 0.45 K and a $T_c=0$ superconducting energy gap of 0.10 meV that are associated with the Ru microdomains. The systematic behavior observed in the tunneling spectra, including the presence of a Josephson coupling between In and Ru, a zero bias conductance peak (ZBCP), an unusually large magnitude and the temperature and magnetic field dependences of the superconducting energy gap, suggests that both s- and p-wave pairings are present simultaneously in the interior of a Ru microdomain. We propose the existence of a novel superconducting state featuring the mixing of the s- and the p-wave pairings in this unique superconducting system and discuss the properties of this mixed pairing state.

10:48AM X8.00013 Influence of Hydrostatic Pressure on Magnetoacoustic Properties of Sr$_2$RuO$_4$. O. SVITELSKY, S. HEADLEY, S. TOZER, E. PALM, T. MURPHY, A. SUSLOV, National High Magnetic Field Laboratory, Tallahassee, FL 32310, D. SHULYATEV, Moscow State Institute of Steel and Alloys, Russia 119049 — The interest in the nanolayered Sr$_2$RuO$_4$ crystal is due to its unconventional spin-triplet superconductivity. We used ultrasonic pulse-echo technique to obtain further insight into its electronic structure. We investigated longitudinal 30-300 MHz sound wave propagating in [100] direction of the single crystal Sr$_2$RuO$_4$, grown by floating zone technique, at temperatures down to 300 mK, in magnetic fields up to 18 Tesla, and under hydrostatic pressures up to 7.3 kbar. The decent quality of the material was confirmed by the $T_c$ value of 1.25 K. Under the hydrostatic pressure, $T_c$ and $H_{c1}$ decreased, the superconducting transition width increased, and the sound speed increased. Data analysis allowed us to separate electron and phonon contributions in the sound attenuation.

Session X9 DMP: Superconductivity: Electronic Transport Measurements of Copper Oxide Superconductors  Colorado Convention Center Korbel 1D

Friday, March 9, 2007 8:00AM - 10:36AM

8:00AM X9.00001 ABSTRACT WITHDRAWN

8:12AM X9.00002 Quantum superconductor-to-insulator transition in 2D $Y_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$ films. IULIAN HETEL, THOMAS LEMBERGER, Department of Physics, The Ohio State University, Columbus, Ohio. 43210 — This study investigates the relationship between the critical temperature, $T_c$, and the zero temperature superfluid density, $n_s(0)$, close to the quantum superconductor-to-insulator transition in 2D cuprate films. We use a two-coil technique, at frequencies up to 50 kHz, to measure the temperature dependence of superfluid density in severely underdoped $Y_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$ films, as thin as 1-2 unit cells and with transition temperatures as low as 3K. Superconducting films are grown by pulsed laser deposition on SrTiO$_3$ substrates, with thick insulating PrBa$_2$Cu$_3O_{7-\delta}$ protecting the film above and below. The zero temperature superfluid density in these films is comparable to values measured in thicker $Y_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$ films, which suggests continuous superconducting layers. In 1-2 unit cell thick films, we find $T_c \propto n_s(0)$, which is expected in 2D. This result is different from the approximate $T_c \propto n_s(0)^{1/2}$ dependence previously reported in $YBa_2Cu_3O_{7-\delta}$ films and crystals and confirmed by our measurements on thicker $Y_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$ films.

8:24AM X9.00003 Exploring the critical dynamic exponent using YBCO films and untwinned crystal in zero and non-zero magnetic field. SU LI, HUA XU, STEVEN M. ANLAGE, C. J. LOBB, University of Maryland, College Park — The phase transition in high Tc superconductors in zero and non-zero magnetic field has been intensely studied. However, there are debates on the critical dynamic exponent $z$ from both simulations and experiments. We will report our result on $z$ from our dc transport measurement in both YBCO films and untwinned crystals. Our results show that the finite size effects, which can cause misinterpretation in the film data, are absent in the crystal data, and the data on both the films and crystals give a very similar result for the critical dynamic exponent. (This work was supported by NSF grant number DMR-0302596)

8:36AM X9.00004 Upper critical field in electron-doped Pr$_{2-x}Ce_xCuO_4$ in parallel magnetic fields. PENGCHENG LI, Center for Superconductivity Research and Department of Physics, University of Maryland, College Park, MD 20742, F.F. BALAKIREV, NHMFL-LANL, Los Alamos, NM 87545, R.L. GREENE, Center for Superconductivity Research and Department of Physics, University of Maryland, College Park, MD 20742 — We report a comprehensive study of the resistive superconducting transition in the electron-doped Pr$_{2-x}Ce_xCuO_4$ films down to 1.5K for magnetic field up to 58T applied parallel to the conducting ab-planes. We find that the parallel critical field ($H_{c2//ab}$) exceeds 58T for underdoped and optimally doped films. For the overdoped films, 58T is sufficient to suppress the superconductivity. An $H_{c2//ab}$ - T phase diagram is established. A comparison between our experimental results and theories for orbital and spin pairbreaking effects will be presented.

1Sponsored by the NSF Cooperative Agreement No.DMR-0084173, NHMFL-IHRP, and NNSA/DOE.
8:48AM X9.00005 T. suppression and resistivity in cuprates with out-of-plane defects. SIEGFRIED GRASER, Institut fuer Theoretische Physik, Universitaet Tuebingen, Tuebingen, Germany / Physics Department, University of Florida, Gainesville, FL 32611 USA, THOMAS DAHM, Institut fuer Theoretische Physik, Universitaet Tuebingen, Tuebingen, Germany, PETER J. HIRSCHFELD, LINGYIN ZHU, Physics Department, University of Florida, Gainesville, FL 32611 USA — The suppression of the critical temperature due to isotropic impurity scattering in a d-wave superconductor is expected to be described by the Abrikosov-Gor'kov formula. However recent experiments on cuprate superconductors with out-of-plane defects show a nearly linear dependence of the critical temperature as a function of the residual resistivity in contradiction to the Abrikosov-Gor'kov result. Our experiments suggest further that the Tc suppression is stronger for out-of-plane than for in-plane impurities. Both results can be explained assuming that elastic forward scattering is the dominant scattering process for out-of-plane disorder. We present a simple model of forward scattering allowing an analytical solution that already includes the key features of Tc suppression for out-of-plane defects. We also verify the intuitive result of this simple model by comparing it to numerical calculations assuming randomly distributed out-of-plane defects and a realistic band structure appropriate for YBCO.

9:00AM X9.00006 c-axis magnetotransport and noise in underdoped La2−xSrxCuO41, I. RAIC’EVIČ, Dept. of Physics and National High Magnetic Field Laboratory (NHMFL), Florida State Univ. (FSU), J. JAROSZYŃSKI, NHMFL, D. POPOVIC, NHMFL and Dept. of Physics, FSU, G. JELBERT, C. PANAGOPoulos, Cavendish Laboratory, Univ. of Cambridge, T. SASAGAWA, GLAM / Dept. of Appl. Phys., Stanford Univ. — We report a study of c-axis magnetotransport and noise on high quality single crystals of La2−xSrxCuO4 (x = 0.03). The measurements were performed at temperatures 0.11 ≤ T ≤ 50 and fields 0 ≤ B(T) ≤ 1 T parallel and perpendicular to the c axis. Our experiments have revealed for the first time a number of glassy features in the charge response at very low Tc, such as memory effects and history dependence. In the same Tc range, we have observed positive magnetoresistance (MR), which exhibits hysteretic behavior. The hysteretic effects decrease with increasing Tc and vanish at ~ 1.5 K. The crossover from positive to negative MR takes place at higher Tc and Bi. We also have observed switching fluctuations in the time-dependent resistance at the lowest Tc, with switching times varying from several minutes to several hours. The possible origins of the observed glassiness will be discussed.

1Supported by NSF Grant No. DMR-0403491, NHMFL through NSF Cooperative Agreement No.DMR-0084173, and The Royal Society.

9:12AM X9.00007 Pulsed laser deposition growth and transport studies of superconducting La1.85Y0.15CuO4 thin films. WEIQIANG YU, B. LIANG, P. LI, R. L. GREENE, Center for Superconductivity Research, Department of Physics, University of Maryland, College Park, MD 20742, S. FUJINO, T. MURAKAMI, I. TAKEUCHI, Department of Material Science and Engineering, University of Maryland, College Park, MD 20742 — The recent MBE growth of the “nominally undoped” cuprate superconductor (La1.85RE0.15CuO4) has led to the speculation that this system is a band metal and not a “doped Mott insulator” as found in all other superconducting cuprates. We report the first pulsed laser deposition (PLD) growth of insulating and superconducting La1.85Y0.15CuO4 thin films, which are prepared under different oxygen conditions. We also report resistivity, Hall, Nernst, and magnetoresistance measurements, which show that La1.85Y0.15CuO4 is an electron-doped, Mott-insulator system, where the carriers originate from oxygen nonstoichiometry produced by the oxygen reduction. This work is supported by NSF (DMR 0352735).

9:24AM X9.00008 Superconducting Phase Diagram and Vortex-glass Scaling of the Electron-Doped Superconductor Sm2−xCexCuO4−y. D.J. SCANDERBEG, B.J. TAYLOR, R.E. BAUMBACH, K.T. CHAN, M.B. MAPLE, University of California, San Diego — We report the growth and characterization of thin films of the electron-doped superconductor Sm2−xCexCuO4−y over a wide doping range 0.13 ≤ x ≤ 0.19. The shape of the superconducting dome is similar to other electron-doped compounds, such as Nd2−xCexCuO4−y and Pr2−xCexCuO4−y, and shows a peak in the superconducting transition temperature Tc at a doping level x ≈ 0.15. Magnetoresistance data ρ(H, T) in fields up to 17 T reveal a metal to insulator transition in the underdoped region. Analysis of Hall effect measurements from the underdoped to overdoped regime is presented along with vortex-glass (VG) scaling analysis of the transport measurements. VG scaling shows no change in the dynamical vortex behavior from the underdoped to overdoped regions. This research was sponsored by the DOE under Grant No. DE-FG02-04ER46105 and the CULAR program no. 9985-001. A portion of this work was performed at the National High Magnetic Field Laboratory (NHMFL), which is supported by NSF Cooperative Agreement No. DMR-0084173, by the State of Florida, and by the DOE.

9:36AM X9.00009 Metal-insulator transition in YBa2Cu3Oδ. LOUIS TAILLEFER, Universite de Sherbrooke and Canadian Institute for Advanced Research, CYRIL PROUST, LNCMP Toulouse, NICOLAS DOIRON-LEYRAUD, Universite de Sherbrooke, MIKE SUTHERLAND, University of Cambridge, D. LE BOEUF, Universite de Sherbrooke, LEVALLOIS, M. NARDONE, LNCMP Toulouse, H. ZHANG, University of Toronto, N. HUSSEY, University of Bristol, S. ADACHI, International Superconductivity Center, RUIXING LIANG, D.A. BONN, W.N. HARDY, University of British-Columbia and CIAR — The non-superconducting ground state of the underdoped cuprates YBa2Cu3Oδ and YBa2Cu4O6 was examined by measuring the electrical resistivity of high-quality single crystals in magnetic fields up to 60 T. A metal-insulator-like crossover is observed near a critical doping p = 0.1, i.e., far in the underdoped region. This shows that the pseudogap phase present below Tc is a metal, characterized by a resistivity of the Fermi-liquid form, ρ0 + Atp, where ρ0 is small, just as in the strongly overdoped regime. In the metallic phase, the transverse magneto-resistance undergoes a qualitative change between p = 0.14, where it saturates at high field, and p = 0.11, where it does not saturate. This would suggest that a change in the nature of the ground state occurs in the vicinity of p = 1/8.

9:48AM X9.00010 The Effect Of hBN addition on properties of Bi-2223 superconductors. MUSTAFA AKDOGAN, ERHAN BUDAK, OZGUR OZTURK, CABIR TERZIOLGU, IBRAHIM BELENLI, Abant Izzet Baysal University — The effect of the addition of hBN (x = 0.005, 0.015, 0.025, 0.035 and 0.05 g.) in the Bi-2223 superconducting samples have been investigated in terms of magnetoresistivity, Tc, Jc, and ac susceptibility. The samples were prepared by the conventional solid-state reaction method. We estimated the transition temperature, the activation energy values of the samples from the resistivity vs. temperature measurements in dc magnetic fields up to 0.7 T. We observed that transition temperature, Tc, and transport critical current density, Jc, depend on the hBN addition. They both decrease with increasing x up to 0.025 g. With further increasing x up to 0.035 g. Activation energy, U0, is calculated from resistivity versus temperature at various magnetic fields. It is observed that U0 depend on both the hBN content of samples and the applied magnetic field. The ac susceptibility measurements were carried out at different values of the ac magnetic field amplitudes up to 555 A/m. The imaginary part of ac susceptibility measurements is used to calculate Jc, using the Bean’s Model. The intergranular critical current density is also seen to vary with increasing hBN content. We extracted the peak temperature, Tp, and the pinning force density from our previous ac susceptibility measurements. The pinning force density varied with increasing the hBN content of samples.
10:00AM X9.00011 Investigation of some physical properties of gold diffusion-doped Bi$_1$$_x$Pb$_3$Sr$_{1-y}$Ca$_2$Cu$_3$O$_7$ superconductors, OZGUR OZTURK, Abant Izzet Baysal University, MUSTAFA YILMAZLAR, Sakarya University, TAYFUR KUCUKMEROGLU, Karadeniz Technical University, USMAN GORUR, Rize University, CABIR TERZIOGLU, Abant Izzet Baysal University. We have studied the effect of the gold-diffusion doped Bi-2223 superconducting samples on the crystal structure and superconducting properties using XRD, SEM, T$_c$, J$_c$, and room temperature resistivity measurements. Doping of Bi-2223 was carried out by means of gold diffusion from an evaporated onto pellets at the sintering. XRD patterns and SEM micrographs are used to obtain information about Bi-2223 phase ratio, lattice parameters calculations and grain size, respectively. The gold diffusion in the Bi$_1$$_x$Pb$_3$Sr$_{1-y}$Ca$_2$Cu$_3$O$_7$ has been also studied over the temperature range 500-800 $^\circ$C using the technique of successive removal of thin layers and measurement of the sample resistivity at room temperature. The temperature dependence of the Au diffusion coefficient in the range 500-800 $^\circ$C was described by the relation D=4x10$^{-4}$exp(-1.08 eV/kBT). For the Au-doped sample, the critical transition temperature and J$_c$ were increased from 100 K to 104 K and from 40 to 125 A cm$^{-2}$, respectively, in comparison with those of undoped Bi-2223. The possible reasons for the observed increases in critical temperature and critical current density due to Au diffusion were discussed.

10:12AM X9.00012 The effect of Sm substitution on properties of Bi$_1$$_x$Pb$_3$Sr$_{2-y}$Ca$_2$Cu$_3$O$_7$ superconductors, HUSEYIN AYDIN, Abant Izzet Baysal University, MUSTAFA YILMAZLAR, Sakarya University, OZGUR OZTURK, DINCER YEGEN, CABIR TERZIOGLU, Abant Izzet Baysal University. The effect of the partial substitution of Ca by Sm in the Bi-2223 superconducting samples have been investigated in terms of XRD, magnetoresistivity, critical temperature, transport critical current density, and ac susceptibility. The samples were prepared by the conventional solid-state reaction method. XRD patterns are used to calculate lattice parameters and obtain about Bi-2223 phase ratio. The volume fraction was determined from the intensities of Bi-2223 and Bi-2212 peaks. The room temperature XRD patterns of the samples showed the presence of Bi-2223 phase decreases with increasing the Sm content. We estimated the transition temperature, the activation energy values of the samples from the resistivity vs. temperature measurements in dc magnetic fields up to 0.6 T. We observed that transition temperature, T$_c$, and transport critical current density, J$_c$, depend on the Sm substitution. They both decrease with increasing the Sm substitution. Activation energy, U$_0$, is calculated from resistivity versus temperature at various magnetic fields in both high temperature region and low temperature region. It is observed that U$_0$ depend on both the Sm content of samples and the applied magnetic field.

10:24AM X9.00013 Orientation and Grain Boundaries in Bulk Samples of Bi-2223 Phase, MURAT ERDEM, OZGUR OZTURK, CABIR TERZIOGLU, IBRAHIM BELENLI, Abant Izzet Baysal University. In polycrystalline high-T$_c$ compounds the critical current densities are mostly limited by the grain boundaries. Their characterization is of significant importance to understand and improve the superconducting properties. In our work, superconducting Bi$_1$$_x$Pb$_3$Sr$_{1-y}$Ca$_2$Cu$_3$O$_7$ samples were prepared by the standard solid-state reaction method. 20 samples were tested in pellets and optimum annealing temperatures were found as 835$^\circ$C for the first annealing and 830$^\circ$C for the second annealing respectively. The optimum Between the first and second annealing procedure, the pellets are pressed piled up. After the second annealing, six bar samples were cut, three of them were perpendicular and the others parallel to the pressing surface. The transport T$_c$ and J$_c$ were measured using standard four-probe method. Micro structural examination of the samples were done using SEM. Degrading effect of the magnetic field on J$_c$ is much more significant for the perpendicular sample. This is in agreement with literature and ensures that our samples had preferred orientation. We have proved that preferred orientation in bulk pellet samples of (Bi, Pb)-2223 phase can be achieved by the method described in this work. Orientation of the magnetic field with respect to grain boundaries may be an important issue for transport critical current values in applied magnetic fields.

Friday, March 9, 2007 8:00AM - 10:48AM

Session X12 GMAG DMP FIAP: Focus Session: Anomalous Hall Effect and Spin Orbit Coupling

Colorado Convention Center Korbel 3C

8:00AM X12.00001 A Tunable Anomalous Hall effect in a Non-Ferromagnetic System, JOHN CUMINGS, University of Maryland. — The anomalous Hall effect (AHE) is a ubiquitous signature of ferromagnetism that has been known for almost as long as the Hall effect itself. Despite this, its theoretical origins nevertheless remain a subject of debate. In recent years, the physics behind the AHE has been employed to control spin transport in non-magnetic conductors via its sister phenomenon, the spin Hall effect (SHE). In this talk, I will present measurements of a magnetically-doped semiconductor quantum well that reveal a robust and tunable AHE, despite the absence of ferromagnetism. I will show that the AHE can be tuned in-situ by the application of a voltage to a nearby gate electrode and that this helps to uncover the origins of the effect. Most surprising is the fact that the parent material, ZnSe, is known to have only weak spin-orbit coupling, a property usually believed to be required for a strong AHE or SHE. This suggests that controllable semiconductor spin-transport might be realized in a larger class of materials than previously thought. Collaborators: L. S. Moore, H. T. Chou, K. C. Ku, G. Xiang, S. A. Crooker, N. Samarth, and D. Goldhaber-Gordon. See PRL 96, 196404.

8:36AM X12.00002 Anomalous Hall Effect and Anomalous Nernst Effect in Ga1-xMnxAs, YONG PU, JING SHI, Department of Physics, University of California-Riverside. DAICHI CHIBA, FUMIHIRO MATSUKURA, HIDEO OHNO, RIEC, Tohoku University, Japan — We have carried out systematic electrical and thermoelctic transport coefficient measurements on a series of Ga1-xMnxAs samples (x from 0.01 to 0.07) with perpendicular magnetic anisotropy. 50 nm-thick Ga1-xMnxAs films were grown by molecular beam epitaxy on an InGaAs buffer layer with a tensile strain to induce the perpendicular anisotropy. Below the Curie temperature, we have observed a non-zero transverse thermopower Sxy that accompanies the Hall resistance Rxy. Both Sxy and Rxy show abrupt jumps as the magnetization switches by an external magnetic field. Despite this, its theoretical origins nevertheless remain a subject of debate. In recent years, the physics behind the AHE has been employed to control spin transport in non-magnetic conductors via its sister phenomenon, the spin Hall effect (SHE). In this talk, I will present measurements of a magnetically-doped semiconductor quantum well that reveal a robust and tunable AHE, despite the absence of ferromagnetism. I will show that the AHE can be tuned in-situ by the application of a voltage to a nearby gate electrode and that this helps to uncover the origins of the effect. Most surprising is the fact that the parent material, ZnSe, is known to have only weak spin-orbit coupling, a property usually believed to be required for a strong AHE or SHE. This suggests that controllable semiconductor spin-transport might be realized in a larger class of materials than previously thought. Collaborators: L. S. Moore, H. T. Chou, K. C. Ku, G. Xiang, S. A. Crooker, N. Samarth, and D. Goldhaber-Gordon. See PRL 96, 196404.

8:48AM X12.00003 Sign change of anomalous Hall coefficient with temperature in Ga1-xMn2Sb random alloys, M. EGINLIGIL, B. G. KIM, H. LUO, B. D. MCCOMBE, SUNY Buffalo — We have observed sign changes as a function of temperature (T) in the anomalous Hall (AH) coefficient of ferromagnetic (FM) Ga1-xMn$_x$Sb films showing weakly localized behavior in the electrical transport. Low magnetic field measurements vs. T (below the Curie temperature, T_C, which is between 13K and 24K) show changes in the sign of the slope of the AH resistance vs. field. We attribute this unusual behavior to the movement of the chemical potential (μ) through the density of states (DOS) extrema in the spin dependent impurity band(s) as recently predicted theoretically [1]. We have developed a model based on the prediction that the AH coefficient depends on the local slope of the DOS in the hopping conduction regime. Our model uses the experimentally determined hole and Mn$^{2+}$ concentrations to find the position of the μ vs. T. The two spin dependent impurity bands in the FM state are assumed to be gaussian. Below T_C, with increasing T, the spin-up and spin-down impurity bands move towards the energy gap and overlap. As T increases μ moves from its initial position on the positive slope of the low energy band (EB) through the minimum before continuing across the maximum of the higher EB. This analysis is in qualitative agreement with our experimental results. [1] Burkov and Balents, PRL, 91 (2003) Supported by NSF ESC 0224206 and University at Buffalo, SUNY.
We also show that the ferromagnetic coupling between localized Mn moments exhibits a strong real space anisotropy. The Mn ions enhances the spin polarization. This is primarily because the additional field from the ferromagnetically aligned impurities polarizes the itinerant carriers. We find that while spin-orbit coupling reduces the spin polarization by mixing different spin states in the valence bands, disorder from the random locations of Mn ions affects the carrier polarization? Using a realistic multi-band tight-binding model with disorder effects included exactly, we find upon examining the system are discussed.

The work is supported by ONR Grant N00014-06-1-0616

The anomalous Hall effect (AHE) is observed in the system, the Hall conductivity (AHC) which is valid for any damping rate $\frac{\hbar}{2}\tau$. This expression enables us to calculate the AHC in metals with a wide range of resistivity $\rho$. The obtained AHC is almost constant with a value of $10^3 \sim 10^4\Omega^{-1}\text{cm}^{-1}$ when $\rho$ is small, as found by Karplus and Luttinger. However, this relation does not hold any more in bad metals; we show that AHC is proportional to $\rho^{-2}$ when $\hbar/2\tau$ is larger than the minimum band-splitting measured from the Fermi level, $\Delta$. This crossover behavior of the intrinsic AHE, which was first derived by H. Kontani and K. Yamada [J. Phys. Soc. Jpn. 63 (1994) 2627], is recently observed in various ferromagnetic metals universally by A. Asamitsu et al. We also present the mechanism of spin hall effect in transition metal oxides.

The limitations of AHE as a tool to test the intrinsic nature of ferromagnetism in a diluted magnetic system. Possible reasons for the origin of the AHE in our system is established by several protocols of magnetic measurements. Nevertheless, the anomalous Hall effect (AHE) is observed in the system, the Hall resistivity vs magnetic field loops being found to be identical to the magnetic hysteresis loops. This once again (Phys. Rev. Lett. 92, 166601 (2004)) highlights the limitations of AHE as a tool to test the intrinsic nature of ferromagnetism in a diluted magnetic system. Possible reasons for the origin of the AHE in our system are discussed.
8:00AM X13.00001 Nonthermal Photoresponse in Epitaxial Thin Films of (La,Pr)$_{67}$Ca$_{33}$MnO$_4$: Correlation with Non-ohmic Electrical Transport and Magnetoresistance. ANTHONY DAVIDSON III, RAJESWARI KOLAGANI, GRACE YONG, VERA SMOLYANINOVA, Towson University, MASON OVERBY, Towson University (Currently at Purdue University) — We have recently observed a non-thermal component of light induced resistance change in the vicinity of the insulator-metal transition in epitaxial films of the manganite material (La$_{67}$Pr$_{33}$)$_{67}$Ca$_{33}$MnO$_4$ (LPCMO). LPCMO is known to have the co-existence of insulating and metallic regions. On cooling, the metallic regions grow at the expense of the insulating regions, giving rise to a percolative insulator-metal transition. Our results indicate that light may cause electronic changes in the insulating regions thus decreasing the electrical resistance. We will present our studies of the photoresponse and the correlation of the observed non-thermal photoresponse with magnetoresistance as well as current-voltage (I-V) characteristics. I-V measurements show that there is a current induced change in resistance which is not due to the Joule heating effects. This effect is only seen in the metal-insulator transition range of the samples, similar to the nonthermal photoresponse, suggesting a common origin for these two phenomena. The effects of magnetic field however are seen to be distinct. A large magnetoresistance is seen at lower temperatures where the light and current induced effects are absent, thus suggesting a very different physical origin for the magnetoresistance.

8:12AM X13.00002 Evolution of the CO-OO and AF ordering in the single-layer manganite Pr$_{1-x}$Ca$_{1+x}$MnO$_3$ near half doping. FENG YE, J. A. FERNANDEZ-BACA, Oak Ridge National Lab., SONGXUE CHI, PENGCHENG DAI, Univ. of Tennessee, Knoxville, J. W. LYNN, NIST Center for Neutron Research, R. MATHIEU, Y. KANEKO, ERATO-SSS, Y. TOKURA, Univ. of Tokyo — Manganese oxides have attracted considerable attention due to the CMR effect observed in the perovskite manganite $A_1_xA'_2$MnO$_3$ near $x = 0.3$. A peculiar charge/orbital (CO-OO) accompanied by antiferromagnetic (AF) order occurs when the carrier concentration is close to half doping ($x = 0.5$). To understand the interplay between the charge, lattice and spin degrees of freedom in such insulating state, we used elastic neutron scattering to study the evolution of the CO-OO and AF order. $A$ = Pr, Sr, Ca. In Pr$_{1-x}$Ca$_{1+x}$MnO$_3$, we find that even in the absence of Jahn-Teller distortions, this compound is strongly orbitally ordered. Fitting of the Mn $L_2$ and $L_3$ edge resonant soft-x-ray magnetic scattering to Study Dynamics in the CMR Manganites indicates that even in the absence of Jahn-Teller distortions, this compound is strongly orbitally ordered. Fitting of the Mn $L_2$ and $L_3$ edge resonant soft-x-ray magnetic scattering to Study Dynamics in the CMR Manganites.

8:16AM X13.00003 Dimensional Crossover of Antiferromagnetism in Half-Doped La$_{0.5}$Sr$_{1.5}$MnO$_4$. KUO-SHENG CHAO, National Chiao-Tung Univ., Taiwan, J. OKAMOTO, D. J. HUANG, National Synchrotron Radiation Research Center, Taiwan, C. Y. MOU, National Tsing Hua Univ., Taiwan, H. -J. LIN, C. -H. HSU, National Synchrotron Radiation Research Center, Taiwan, Y. KANEKO, R. MATHIEU, Spin SuperStructure Project, Japan, Y. TOKURA, Univ. of Tokyo, Japan, C. T. CHEN, National Synchrotron Radiation Research Center, Taiwan — Like cuprates which exhibits high-temperature superconductivity, half-doped single-layered manganites such as La$_{0.5}$Sr$_{1.5}$MnO$_4$ have distinct features of the MnO$_2$ plane in the perovskite structure. In addition to charge-orbital order, of particular interest is the antiferromagnetism in half-doped manganites with the so called CE-type antiferromagnetic (AF) structure which is essentially composed of ferromagnetic zigzag chains antiferromagnetically coupled to one-another. In this talk, we will report critical behavior and dimensional crossover of AF order in La$_{0.5}$Sr$_{1.5}$MnO$_4$ based on measurements of resonant soft-x-ray magnetic scattering. A 2D incommensurate AF order exists at temperatures above the Neel temperature $T_N$. As the temperature cools across $T_N$, the interlayer exchange coupling prevails and the 2D incommensurability collapses to stabilize the 3D AF order. The measurements unravel spin correlations in the classical renormalized region for a non-standard (CE-type) antiferromagnet.

8:36AM X13.00004 Role of oxygen in the orbital ordered state of La$_{0.5}$Sr$_{1.5}$MnO$_4$. J. W. FREELAND, Advanced Photon Source, Argonne National Laboratory, MICHEL VAN VEEENDAAL, Department of Physics, Northern Illinois University, KEN GRAY, QING'AN LI, HONG ZHENG, JOHN F. MITCHELL, Materials Science Division, Argonne National Laboratory — In the single layer manganite, La$_{0.5}$Sr$_{1.5}$MnO$_4$, experimental evidence points clearly to formation of orbital ordering but leaves the question open as to the exact nature of the state. Using oxygen K edge resonant soft-x-ray magnetic scattering, we find that oxygen holes related to the Mn-O hybridization between O($\alpha$) and Mn($\epsilon$) states play an important role in the formation of the ordered groundstate. The large change in the number of $e_g$ related oxygen holes with the formation of the charge/orbital ordered states demonstrates it is not due to a locking in of orbitals which are fluctuating in orientation, but that the disordered state possesses a different orbital occupancy. The change in the number of $e_g$ holes occurs mainly within the ab plane and seems to be related to the crossover from ferromagnetic to antiferromagnetic correlations with the onset of the charge/orbital ordered state. This idea is supported by MnO$_2$ cluster calculations. Work at Argonne is supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

8:48AM X13.00005 Orbital Ordering in Magnanites Probed with Soft X-Ray Scattering. STUART WILKINS, Brookhaven National Laboratory, NATASA STOJIC, Abdus Salam International Centre for Theoretical Physics, THOMAS BEALE, University of Durham, NADIA BINGELI, Abdus Salam International Centre for Theoretical Physics, PETER HATTON, University of Durham, D. PRABHAKARAN, ANDREW BOOTHROYD, University of Oxford, MASSIMO ALTARELLI, Abdus Salam International Centre for Theoretical Physics — Orbital ordering is important in the understanding of transition metal oxides as the magnetic and transport properties are strongly related to the orbital and charge degrees of freedom. In the case of La$_{0.5}$Sr$_{1.5}$MnO$_4$ we will present results using diffraction at the L-edges of Mn, for the orbital order superlattice reflection, and show that while that there indeed does exist long range order of the orbitals the dominant transport property is cooperativity. By comparing these measurements with theoretical calculations we find that the dominant orbital ordering of the $d_{x^2-y^2}$ type, in contrast to the $d_{xy}$ type as previously proposed. In La$_{0.5}$Sr$_{1.5}$MnO$_2$, which is found crystallographically to have virtually no Jahn-Teller distortion of the oxygen octahedra. We will show that even in the absence of Jahn-Teller distortions, this compound is strongly orbitally ordered. Fitting of the Mn L-edge resonance spectra demonstrates the presence of orbital ordering of the Mn$^{3+}$ ions within an almost cubic crystal field.

9:00AM X13.00006 Rethinking the Orbital Ordering Transition: Using Coherent Soft X-ray Scattering to Study Dynamics in the CMR Manganites. JOSHUA TURNER, University of Oregon and Advanced Light Source, JESSICA THOMAS, JOHN HILL, Brookhaven Lab, MARK PFIEFFER, University of Oregon and Advanced Light Source. KARINE CHESNEL, Advanced Light Source, JESSICA THOMAS, JOHN HILL, Brookhaven Lab, MARK PFIEFFER, University of Oregon and Advanced Light Source. KARINE CHESNEL, Advanced Light Source — The colossal magnetoresistance (CMR) phenomenon has baffled physicists since its discovery over a decade ago. Central to the puzzle is the short-range orbital ordering that arises in certain high concentrations of the manganese oxides, even for low temperatures. We have used a Coherent Soft X-ray Scattering (CSXS) technique to resonantly enhance the orbital ordering contrast and measure speckle patterns from the domain structure of the self-assembling Mn d-orbitals. Our dynamics measurements suggest that the orbital domains remain static through the orbital ordering transition temperature — challenging the previous belief of a mediation through slow, glass-like characteristics. Our experiments force us to rethink the role and nature of the orbital-ordered state in the manganites, intrinsic to CMR.
9:12AM X13.00007 Resonant soft x-ray scattering study on antiferromagnetic ordering of La\(_{2-\delta}\)Sr\(_{\delta}\)Mn\(_2\)O\(_7\). — J.-S. LEE, J. KOO, H. JANG, K.-T. KO, H. J. LEE, Y. H. JEONG, K.-B. LEE, J.-H. PARK, eSSC and Dept. of Physics, POSTECH, J.-Y. KIM, Y. BANG, Dept. of Physics, Chonnam National University, T. KIMURA, Y. TAKURA, Dept. of Applied Physics, University of Tokyo — Resonant soft x-ray scattering experiments at the Mn \(L_{2,3}\) edge and O \(K\)-edge have been performed to probe the magnetic structure of La\(_{2-\delta}\)Sr\(_{\delta}\)Mn\(_2\)O\(_7\) which is well known as the \(A\)-type antiferromagnetic (AFM) phase. At the low temperature, strongly resonant intensity of (001) AFM reflection was found. The temperature dependences of AFM resonance at both the Mn \(L_{2,3}\) and O \(K\)-edge were relatively different, in which the order parameter at Mn \(L_{2,3}\)-edge showed an anomalous transition above \(Ne\)-el temperature (170 K). This feature could be regarded as the mixed valence state (Mn\(^{3+}\) and Mn\(^{4+}\)) phenomenon, and besides, it could be supported by theoretical calculation and bulk measurement on magnetism. Detailed description will be discussed in presentation.

1Pohang Accelerator Laboratory and POSTECH

9:24AM X13.00008 Reentrant orbital order and the true ground state of La\(_{2}\)Sr\(_{2}\)Mn\(_2\)O\(_7\). — S. NYBOR ANCONA, S. ROSENKRANZ, R. OSBORN, K. E. GRAY, H. ZHENG, QING'AN LI, J. F. MITCHELL, Materials Sciences Division, Argonne National Laboratory, Argonne, IL 60439, U.S.A.; Y. CHEN, J. LYNN, NIST Center for Neutron Research, Gaithersburg, MD 20899, U.S.A. — Strongly correlated electron systems, and colossal magnetoresistive materials, exhibit a strong competition among orbital, charge and spin order. The phase diagram of the bilayer manganites, La\(_{2-x}\)Sr\(_{1+x}\)Mn\(_2\)O\(_7\), display interesting features near half doping, \(x \approx 0.5\), and it has been commonly accepted that CE order at \(x = 0.5\) is reentrant. Here, we present x-ray and neutron diffraction data of our purified La\(_{2-x}\)Sr\(_{1+x}\)Mn\(_2\)O\(_7\) crystals contrasting the conventional wisdom. Our crystals exhibit CE-type orbital and charge order as the low-temperature ground state for \(x = 0.5\). For small deviations from \(x = 0.5\), the high temperature CE phase is replaced at low temperatures by an \(A\)-type antiferromagnetic phase without coexistence. Larger deviations from \(x = 0.5\) result in a lack of CE-order at any temperature. Thus small compositional variations could explain why others commonly see this reentrance with coexistence.

9:36AM X13.00009 Exotic Bilayer Manganese Phase Diagram near \(x = 0.6\) Hole Doping, — KENNETH GRAY, HONG ZHENG, QING’AN LI, JOHN F. MITCHELL, STINE NYBOR ANCONA, STEPHAN ROSENKRANZ, RAY OSBORN, Argonne National Laboratory — Important modifications to the phase diagram of the bilayered manganites have been discovered through combined measurements of conductivity, magnetization and neutron and x-ray diffraction. The previously reported phase diagram for the CE-type orbital and charge order in La\(_{2-x}\)Sr\(_{1+x}\)Mn\(_2\)O\(_7\) (near hole doping of \(x = 0.5\)) is qualitatively reproduced and graphically demonstrated for the bi-stripe (BIS) orbital and charge order in La\(_{0.8}\)Sr\(_{1.2}\)Mn\(_2\)O\(_7\) crystals near \(x = 0.6\). Individual crystals, taken along the compositional gradient of a single boule made by the floating-zone technique with nominal composition \(x = 0.6\), display a large fraction of the phase diagram. As in the case of \(x = 0.5\), we find (1) crystals that enter the BIS phase at 240–300 K and reenter into an in-plane metal, A-type antiferromagnetic phase, and (2) crystals that retain BIS order down to at least 5 K. Surprisingly, the BIS state seems somewhat more stable than the CE state.

1This research was supported by the U.S. Department of Energy, Basic Energy Sciences-Materials Sciences, under contract # DE-AC02-06CH11357.

9:48AM X13.00010 Polarized transmission EXAFS study of single crystal La\(_{2-\delta}\)Sr\(_{1+\delta}\)Mn\(_2\)O\(_7\) as a function of temperature, — JESSE GUZMAN, G. KURCZEVI, L. DOWNWARD, F. BRIDGES, UC Santa Cruz, J. MITCHELL, H. ZHENG, Argonne National Lab. — The temperature dependence (3-300K) of the bilayer Colossal Magneto Resistive (CMR) manganites La\(_{2-x}\)Sr\(_{1-x}\)Mn\(_2\)O\(_7\), \(x = 0.34\) and \(0.36\), was studied using polarized, transmission EXAFS through a thin single crystal, with the x-rays polarization parallel to the c-axis or in the ab-plane. To eliminate Bragg diffraction effects from the single crystal, a 2D sample oscillator setup was used; the results of using this oscillator will be discussed. The data analysis shows a sharp increase in the width \(\sigma\) of the pair distribution function (PDF) for the Mn-O peak near the ferromagnetic transition temperature \(T_g\). This sharp increase in \(\sigma^2\) corresponds to a Jahn-Teller-like distortion as the temperature goes through \(T_g\). Furthermore, a plot of the reduction in \(\sigma^2\), \(\Delta(\sigma^2)\), vs. sample magnetization \(M\) shows a linear dependence with a large change in slope at \(M/M_{c} = 0.5\), which is consistent with the recently proposed dimeron model proposed by Downward, et al. with regards to the LCMO system. Furthermore, there is some evidence for an increase in disorder below 75K which has not been discussed previously. Finally, another weaker step in \(\sigma^2\) at \(T^* = 250K\), well above \(T_g\), can be seen, which is comparable to a \(T^*\) in recent neutron scattering experiments, proposed to be a spin-liquid/spin-glass phase transition. Support: NSF DMR0301971.

10:00AM X13.00011 Magnetic momentum density, Fermi surface and directional magnetic Compton profiles in La\(_{2}\)Sr\(_{2}\)Mn\(_2\)O\(_7\) and La\(_{1.5}\)Sr\(_{1.8}\)Mn\(_2\)O\(_7\). — P. E. MIJNARENS, Delft University of Technology and Northeastern U., S. KAPRZYK, Northeastern U., and AGH (Poland); B. BARBIELLINI, A. BANSIL, Northeastern U., YINWAN LI, U. of Illinois Chicago and Argonne Nat. Lab., J. F. MITCHELL, Argonne Nat. Lab.; P. A. MONTANO, U. of Illinois Chicago and USDOE — We have carried out first principles, all-electron computations of the magnetic momentum density \(\rho_{\text{mag}}(p)\) and magnetic Compton profiles (MCPs) for momentum transfer along the [100], [010], and [110] directions in La\(_{2}\)Sr\(_{2}\)Mn\(_2\)O\(_7\) and La\(_{1.5}\)Sr\(_{1.8}\)Mn\(_2\)O\(_7\) \[1\]. Parallel measurements of these three MCPs from a single crystal of La\(_{1.5}\)Sr\(_{1.8}\)Mn\(_2\)O\(_7\) at 5 K in a magnetic field of 7 T are also reported. Here, we discuss details of the FS-related signatures in the first and higher BZs in the MCPs and show that high resolution Magnetic Compton scattering experiments with a momentum resolution of 0.1 a.u. FWHM (full-width-at-half- maximum) or better will be necessary to observe this fine structure. We comment also on the feasibility of using positron annihilation spectroscopy in this connection. Work supported by the USDOE.


10:12AM X13.00012 Optic phonon anomaly as a precursor to polaron formation in a layered CMR manganite. — DMITRY REZNIK, FRANK WEBER, Forschungszentrum Karlsruhe, NADIR ALIOUANE, DIMITRI ARGYRIOU, Hahn-Meitner Institut, MARCUS BRADEN, Physikalisches Institut, Universität zu Köln, WINFRIED REICHARDT, Forschungszentrum Karlsruhe — We found evidence of a precursor effect to polaron formation in the bond stretching phonons in the bilayer CMR manganite La\(_{2-x}\)Sr\(_{1.2}\)Mn\(_2\)O\(_7\) at 10K. Inelastic neutron scattering measurements of these phonons in the XX0 direction show that both the transverse and longitudinal branches broaden abruptly from \(X = 0.15\), where they are resolution limited, to \(X = 0.25\) where FWHM = 13meV. They then narrow again on approach to the zone boundary (X = 0.5). The shell model predicts a downward dispersion following the cosine function for the transverse branch and upward dispersion for the longitudinal branch, which is exactly what is observed in undoped cuprates. But in La\(_{2-x}\)Sr\(_{1.2}\)Mn\(_2\)O\(_7\) both branches show a steep downward dispersion above \(x = 0.15\). The anomalous dispersion and broadening can be understood as a precursor effect to the CMR transition at 125K because they appear at the same wavevectors as the polaron peaks in the same compound observed above 125K near \(q = 0.27\). This behavior is very unusual, but such precursor effects have previously been associated with phase transitions where charge order appears on cooling, not on heating as in CMR manganites.
10:24AM X13.00013 A local metallic state in globally insulating La$_{1-28}$Sr$_{1.70}$Mn$_2$O$_{7}$ well above the metal-insulator transition , ZHE SUN, J. FRASER DOUGLAS, University of Colorado at Boulder, ALEKSI V. FEDOROV, YI-DE CHUANG, Advanced Light Source, Lawrence Berkeley National Laboratory, HONG ZHENG, JOHN F. MITCHELL, Materials Science Division, Argonne National Laboratory, D. S. DESSAU, University of Colorado at Boulder — La$_{1-28}$Sr$_{1.70}$Mn$_2$O$_{7}$ is a typical colossal magnetoresistive oxide, and it shows a drastic transition from a low-temperature metal to a high-temperature insulator at 120K -160K. The famous CMR (colossal magnetoresistive) effect usually accompanies the metal-insulator transition. Using angle-resolved photoemission spectroscopy (ARPES) we studied the electronic structure of a bi-layer manganite compound La$_{1-28}$Sr$_{1.70}$Mn$_2$O$_{7}$ ($x=0.38$). We found that in the insulating state there remain local metallic regions up to a very high temperature. In these metallic regions, the electronic behavior has minimal change with temperature. Our data indicate that the metal-insulator transition is a new type and an "emergent" phenomenon driven by the phase separation and percolation effect. The CMR effect can also be understood in the framework of the phase separation and percolation effect.

10:36AM X13.00014 Angle resolved photoemission studies of colossal magnetoresistive bilayer manganites , NORMAN MANNELLA, WANLI YANG, KIYOHISA TANAKA, XINGJIANG ZHOU, JENNIFER ZHENG, JOHN MITCHELL, JAN ZAANEN, TOM DEVEREAUX, NAOTO NAGOOSA, ZAHID HUSSAIN, ZHI-XUN SHEN, Lawrence Berkeley National Laboratory — In this talk, we will discuss the results of some recent angle-resolved photoemission spectroscopy (ARPES) investigations in the colossal magnetoresistive (CMR) bilayer compound La$_{1-2}$Sr$_1$Mn$_2$O$_7$ (LSMO, $x = 0.4$) [1]. The temperature dependent evolution of the quasiparticle excitations in LSMO has been found to track remarkably well the DC conductivity, thus accounting for the macroscopic transport properties and the metal to insulator transition. Our results indicate that the microscopic mechanism leading to the MIT and the CMR effect in manganites is intrinsically a quantum effect linked to a crossover via the nodal QP collapse from a coherent polaronic conductor in the FM state below T$_C$ to a hopping regime with thermally activated single polarons in the paramagnetic state above T$_C$. The role of the exchange interaction is crucial in controlling the competition between coherence and localization effects. [1] N. Mannella et al., Nature 438, 474 (2005)

10:48AM X13.00015 Energy Range for Coulomb Interaction Effects in La$_{1-28}$Sr$_{1.72}$Mn$_2$O$_{7}$ , DANIEL MAZUR, K. E. GRAY, Argonne National Laboratory, J. F. ZASADZINSKI, Illinois Institute of Technology, L. OZYUZER, Izmir Institute of Technology, I. BELOBORODOV, H. ZHENG, J. F. MITCHELL, Argonne National Laboratory — Tunneling data on La$_{1-28}$Sr$_{1.72}$Mn$_2$O$_{7}$ crystals confirm Coulomb interaction effects through the $\sqrt{E}$ dependence of the density of states (DOS). Importantly, the data and analysis at high energy, E, show conservation of states: those removed from near E_F are found between ~30 and 70 meV from E_F. This quantum correction to the DOS agrees in magnitude with the $\sqrt{E}$ dependence of the bulk conductivity. Combining our results, with published theory and quantum interference data, we find a scattering time and Fermi velocity that agree reasonably well with recent ARPES results.

Friday, March 9, 2007 8:00AM - 10:48AM — Session X14 GMAG DMP FIAP: Focus Session: Spin-Polarized Transport Colorado Convention Center Korbel 4D

8:00AM X14.00001 Tuning the Exchange Bias in Spin Valves by an Electric Current$^1$, MAXIM TSOP$^2$, Physics Department, University of Texas at Austin — An electrical current can transfer spin angular momentum to a ferromagnet. This novel physical phenomenon, called spin transfer, offers unprecedented spatial and temporal control over the magnetic state of a ferromagnet and has tremendous potential in a broad range of technologies, including magnetic memory and recording. Recently, it has been predicted [1] that spin transfer is not limited to ferromagnets, but can also occur in antiferromagnetic materials and even be stronger under some conditions. This talk will discuss our recent experiments [2] that demonstrate the transfer of spin angular momentum across an interface between ferromagnetic and antiferromagnetic metals. The spin transfer is mediated by an electrical current of high density (~1012 A/m2) and revealed by variation in the exchange bias at the ferromagnet/antiferromagnet interface. We find that, depending on the polarity of the electrical current flowing across the interface, the strength of the exchange bias can either increase or decrease. This finding is explained by the theoretical prediction that a spin polarized current generates a torque on magnetic moments in the antiferromagnet. Current-mediated variation of exchange bias could be used to control the magnetic state of spin-valve devices, e.g., in magnetic memory applications. [1] A. S. Nunez, R. A. Duine, P. Haney, and A. H. MacDonald, Phys. Rev. B 73, 214426 (2006). [2] Z. Wei et al., cond-mat/0606462.

$^1$Supported in part by NSF (DMR-06-45377 and DMR-05-01013), DoE (DE-FG03-02ER45958), and the Welch Foundation.

$^2$In collaboration with Z. Wei, A. Sharma, A. S. Nunez, P. M. Haney, R. A. Duine, J. Bass, and A. H. MacDonald

8:36AM X14.00002 Spin transfer in exchange biased magnetic nanopillars, NICKOLAS ANTHONY, SERGEI URAZHIGIN, West Virginia University — We present a study of the effect of current on the magnetic state of nanopatterned ferromagnetic/antiferromagnetic bilayers. We show that the magnetic state of the antiferromagnet can be affected by a high current density. First, the exchange bias can be altered by applying a pulse of current. The change is accompanied by an increase of coercivity. Additionally, the magnetic anisotropy depends on the value and the direction of the applied current. Our findings cannot be explained by the Joule heating, and indicate that a spin transfer effect similar to that previously demonstrated for ferromagnets is also responsible for the current-induced effects in nanopatterned antiferromagnets.

8:48AM X14.00003 Specific Resistance and Scattering Asymmetry of Py/Pd, Fe/V, Fe/Nb, and Co/Pt Interfaces$^1$, AMIT SHARMA, TONY ROMERO, NIKOLETA THEODOROPOULOU, REZA LOLOEE, WILLIAM PRATT JR., JACK BASS, Physics Department, Michigan State University — The properties of interfaces between normal (N) and ferromagnetic (F) metals, described by specific resistance, AR* ($A = $ area, $R = $ resistance), and scattering asymmetry, $\gamma$, are of interest to optimize current-perpendicular-to-plane (CPP) magnetoresistance (MR) and current-induced magnetization-switching (CIMS) in nanopillars. Sputtered standard Py/Cu, Co/Cu, and Fe/Cr interfaces have 2AR* $\sim$ 1 $\Omega$cm and $\gamma \sim 0.7$. Recently, sputtered F/Al interfaces with F = Py, Co, Fe, and Co(91)Fe(9) were found to have very large 2AR* $\sim$ 9 $\Omega$cm, but small $\gamma \leq 0.1$ [1]. In hopes of finding interfaces with both large 2AR* and larger $\gamma$ than for F/Al, we have determined 2AR* and $\gamma$ at 4.2K for sputtered Py/Pd, Fe/V, Fe/Nb, and Co/Pt pairs, where we've matched crystal structures of the F and N metals. We will present our data and our derived values of 2AR* and $\gamma$. [1] N. Theodoropoulou et al., J. Appl. Phys. 99, 085002 (2006); ibid., IEEE Trans. on Magn. (Submitted).

$^1$Supported by NSF Grants DMR 02-02476 and 05-01013.
in-situ we present a first observation of BAMR in Co electrodeposited nanocontacts by scanning tunneling microscope. Here D. JACOB, J. FERNANDEZ-ROSSIER, J.J. PALACIOS, Dpto. de Fisica Aplicada, Universidad de Alicante, Spain — Here we present a method to measure the current-perpendicular-to-plane magnetoresistance (CPP-MR) of a small number of multilayered nanocolumns using a nonmagnetic STM. Samples were grown on Au-coated Si substrates by oblique angle thermal deposition from separate Co and Cu sources. We set the layer thicknesses and column lengths at 5-15 nm and 200-700 nm, respectively. SEM images show column diameters of about 25-100 nm, and the multilayer structure is confirmed by EELS and HR-TEM. VSM analysis gives coercivities of a few tens to several hundred G. In the MR measurement, mechanical contact was established between the STM tip and a small number of as-deposited nanocolumns, and dynamic hysteresis loops of resistance vs. magnetic field (up to 2.5 kG) were then collected in air at room temperature. The observed MR ratio for most samples was on the order of 1%, which is posited to be due to the same physical mechanism as the GMR effect, but with significantly less efficacy. Cautions in the experiment and factors that may facilitate higher MR are also discussed.

9:12AM X14.00005 Large Magnetoresistance in Co/Ni/Co Ferromagnetic Single Electron Transistors1, RUIHENG LIU, HAKAN PETTERSSON, Center for Applied Mathematics and Physics, Halmstad University, Sweden. LUKASZ MICHALAK, CARLO CANALI, Dept of Chemistry and Biomedical Sciences, Kalmar University, Sweden, DMITRY SUYATIN, LARS SAMUELSON, Solid State Physics/the Nanometer Structure Consortium, Lund University, Sweden — We report on magnetotransport investigations of Co/Ni/Co ferromagnetic single electron transistors, fabricated using a high-precision alignment procedure invoked during e-beam writing. As a result of reduced size, the devices exhibit single-electron transistor characteristics at 4.2K. Magnetotransport measurements carried out at 1.8K reveal TMR traces with negative coercive fields, which we interpret in terms of a switching mechanism driven by the shape anisotropy of the central wire-like Ni island. A large TMR of about 18% is observed within a small source-drain bias regime. The TMR decreases rapidly with increasing bias, which we primarily attribute to the excitation of magnons in the central island.

References:

9:24AM X14.00006 Ballistic Anisotropic Magnetoresistance in Electrodeposited Co Nanoco nacts1, ANDREI SOKOLOV, CHUANJUN ZHANG, EVGENY Y. TSYMBAL, JODY REDEPPENING, University of Nebraska-Lincoln, EVGENY KIRIRANOV, Lincoln South-West High School, BERNARD DOUDIN, Institut de Physique et de Chimie des Matériaux de Strasbourg — As dimensions of a metallic conductor is reduced, spin-dependent conductance quantization in units of e²/h leads to unusual magnetoresistive phenomena. One of them is ballistic anisotropic magnetoresistance (BAMR), a quantized change in the ballistic conductance according to the direction of magnetization. Here we present a first observation of BAMR in Co electrodeposited nanoco nacts by in-situ investigation of their spin-dependent transport properties. We compare the results from electrochemically synthesized and break junction contacts. By measuring the conductance as a function of the applied magnetic field direction at saturation, we find the step-wise variation of the ballistic conductance, signature of the BAMR effect. Our results show that BAMR can be positive and negative, and have symmetric and asymmetric angular dependence. This behavior is explained using a simple tight-binding model in terms of the effect of the spin-orbit interaction on the electronic band structure of nanoco nacts.

1 Supported by the Nebraska NRI and the NSF through the MRSEC Program, DMR and CHE depts.

9:36AM X14.00007 ABSTRACT WITHDRAWN —

9:48AM X14.00008 First principles calculations of anisotropic magnetoresistance in ferro magnetic nanocontacts, D. JACOB, J. FERNANDEZ-ROSSIER, J.J. PALACIOS, Dpto. de Fisica Aplicada, Universidad de Alicante, Spain — Here we present ab initio transport calculations of ferromagnetic nanocontacts [1] including the spin-orbit (SO) coupling for the very first time. Due to the SO coupling the conductance of the nanocontact changes with the direction of the magnetization giving rise to the so-called anisotropic magnetoresistance (AMR). We investigate the magnitude of the AMR effect while going from the atomic contact regime (BAMR) [2] to the tunneling regime (TAMR) [3]. Our work is motivated by experiments on 1D/2D/3D magnetic nanocontacts [4,5] which reported much larger AMR values than those usually obtained for bulk materials in agreement with recent electronic structure calculations of ideal monatomic Ni chains [2].

References:

10:00AM X14.00009 Superconductivity suppression by ferromagnetism in bi- and tri-layers of \( \text{La}_{0.7} \text{Ca}_{0.3} \text{MnO}_3 \) ferromagnets and high-\( T_c \) YBa\(_2\)Cu\(_3\)O\(_y\)-based superconductors. NORBERT M. NEMES, FLAVIO Y. BRUNO, MAR GARCIA-HERNANDEZ, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), 28049 Cantoblanco, Madrid, Spain, AXEL HOFFMANN, SUZANNE G. E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, CRISTINA VISANI, CARLOS LEON, ZOUHAIR SERFIOUI, JACOBO SANTAMARIA, GMFC, Departamento de Fisica Aplicada III, Universidad Complutense de Madrid, 28040 Madrid, Spain — Large magnetoresistance occurs in F/S/3 Trilayers of highly spin-polarised \( \text{La}_{0.7} \text{Ca}_{0.3} \text{MnO}_3 \) ferromagnet and high-\( T_c \) superconductor YBa\(_2\)Cu\(_3\)O\(_y\)-based for antiferromagnetic (AF) alignment of the manganite layers. We discuss the relative importance of spin diffusion across the superconductor, proximity effect at the F/S interface and strain fields due to domain walls of the ferromagnet based on magnetoresistance and magnetisation measurements of bilayers and trilayers of various thickness of superconductor and ferromagnet.

10:12AM X14.00010 Spin injection and imbalence in ferromagnet/ superconductor/ ferromagnet double tunnel junctions. HYUNSOO YANG, SEE-HUN YANG, STUAT PARKIN, IBM Almaden research center — The interplay between magnetism and superconductivity can be explored in double tunnel junctions (DTJs) with a superconducting (SC) middle electrode. CoFe/ MGO/ Al/ MgO/ CoFe, prepared using metal shadow masks and magnetron sputter deposition. Due to the strong competition between magnetism and superconductivity induced by the accumulation of spin polarized electrons in the SC, the superconducting gap is reduced with increasing bias voltage for anti-parallel alignment of the two ferromagnetic electrodes, as predicted theoretically [1]. We find that a large inverse (or negative) TMR is observed around gap energy and almost negligible TMR at zero bias. [1] S. Takahashi, H. Imamura, and S. Maekawa, Phys. Rev. Lett. 82, 3911–3914 (1999).
10:24AM X14.00011 Cooper pair phase oscillation in thin Al superconductor induced by effective Zeeman splitting from spin injection\(^1\), GUO-XING MIAO, JOCHEN NIETSCH, JAGADEESH MOODERA, MIT, Francis Bitter Magnet Lab — By placing a superconductor (S) and a ferromagnet (F) in close contact, the superconductivity proximity effect induces Cooper pairs in F leading to FFLO \([1,2]\) state, while the ferromagnetic proximity effect will populate the S region with non-equilibrium parallel spins. In our experiment, the spins are induced from both sides of the superconductor symmetrically through thin Al\(_2\)O\(_3\) tunnel barriers. By toggling the two F layers between parallel and anti-parallel, we can effectively turn on and off the spin imbalance in the Al layer creating > 1000% MR. The Tc of Al layer is shifted between parallel and antiparallel states as a net result of the non-equilibrium spin population. Such Tc shift is observed to oscillate with Al layer thickness, which is a clear evidence that the effective Zeeman splitting caused by parallel spin population can also induce FFLO states in superconductors. The CPP conductance in such a structure also show dramatic difference between the two states. 1. P. Fulde and R.A. Ferrel, Phys. Rev. 135, A550 (1964) 2. A. I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JEPT 20, 762 (1965)\(^1\)

1\(^{\text{Research funded by NSF grant.}}\)

10:36AM X14.00012 ABSTRACT WITHDRAWN —

Friday, March 9, 2007 8:00AM - 10:36AM —

Session X22 GSNP DMP: Focus Session: Deformation and Fracture — Colorado Convention Center 108

8:00AM X22.00001 Crystal strength by direct computation\(^1\), VASILY BULATOV, Lawrence Livermore National Laboratory — The art of making materials stronger goes back to medieval and even ancient times. Swords forged from Damascus steel more than 10 centuries ago possessed a unique combination of hardness and flexibility, two qualities that are difficult to attain simultaneously. The skills of metalworking were based on empirical knowledge and were passed from the master smith to his pupils. The science of physical metallurgy came about only in the XX century bringing with it new methods for finding out why some materials are strong while others are not. Soon it was realized that, when it comes to metal strength, it is all about crystal defects — impurities, dislocations, grain boundaries, etc. and how they are organized into crystal microstructure. This understanding has since resulted in new effective methods of material processing aiming to modify crystal microstructure in order to affect material's properties, e.g. strength and/or hardness. Remarkably and disappointingly, general understanding that microstructure defines material’s response to external loads has not yet resulted in a workable physical theory of metal strength accounting for the realistic complexity of material microstructure. In this presentation I would like to discuss a few tidbits from computational and experimental research in our group at LLNL on crystal defects and their contributions to material strength. My selection of the examples aims to illustrate the major premise of our work that the mechanisms by which the microstructure affects crystal strength are multiple and complex but that there is hope to bring some order to this complexity.

1\(^{\text{This work was performed under the auspices of the US DOE by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.}}\)

8:36AM X22.00002 Modeling of Self-Healing in Materials Reinforced with Nanoporous Fibers\(^1\), VLADIMIR PRIVMAN, Clarkson University — We report on our group’s progress towards continuum rate equation modeling, as well as numerical simulations, of self-healing of fatigue in composites reinforced with glue carrying nanoporous fibers. We conclude that with the proper choice of the material parameters, effects of fatigue can be partially overcome: fracture and degradation of mechanical properties can be delayed.

1\(^{\text{Web site: www.clarkson.edu/Privman}}\)

8:48AM X22.00003 Effects of grain boundary constraints on properties of polycrystalline materials, KIMBERLY MCGARRITY, Dept. of Physics & Astronomy, Michigan State University, ERIN MCGARRITY, Dept. of Chemical Engineering & Materials Science, Michigan State University, PHILLIP DUXBURY, Dept. of Physics & Astronomy, Michigan State University, BRYAN REED, Materials and Technology Division, Lawrence Livermore National Laboratories, ELIZABETH HOLM, Computational Materials Modeling, Sandia National Laboratories — Grain boundary networks are engineered by increasing the fraction of boundaries which have favorable properties. Favorable boundaries have either low grain boundary misorientation or they are special boundaries, such as coincident site lattice boundaries. Significant improvement in properties such as corrosion resistance, critical current in superconductors and mechanical strength and toughness occur, provided percolating grain or grain boundary structures can be engineered. We demonstrate that grain boundary constraints shift percolation thresholds from their uncorrelated values and that the behavior near threshold is also modified. The origin of these behaviors is an enhanced clustering of weak boundaries induced by grain boundary constraints.

9:00AM X22.00004 Modeling the Evolution of Subsurface Microstructures During Wear of Metal Single Crystals\(^1\), CORBETT BATTAILE, SOMURI PRASAD, JOSEPH MICHAEL, Sandia National Laboratories — Friction can lead to complex mechanical and microstructural evolution near the worn surface, and these changes can impact the properties of the material. Recent results from tribological experiments on nickel single crystals reveal the formation of microstructural features ranging from nanometers (very near the surface) to microns in size. The formation and mechanical response of these zones is sensitive to crystallography, and can dramatically alter the frictional properties of the material itself. We have modeled these phenomena using a combination of dislocation plasticity, microstructure formation, and grain boundary sliding. The loading conditions are adopted from an analysis of static frictional contact. A phenomenological treatment of wear debris and asperity-mediated contact is included to appropriately describe the mechanical mixing that occurs near the contact interface. We will provide an overview of the experimental evidence, discuss the wear model in detail, and present results for kilocycle wear on nickel single crystals in different crystallographic orientations.

1\(^{\text{Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.}}\)

9:12AM X22.00005 Spontaneous shear localization in a model brittle solid\(^1\), CRAIG E. MALONEY, MARK O. ROBBINS, Physics and Astronomy, Johns Hopkins — A better understanding of the failure of brittle materials is practically important in situations ranging in scale from nano-indentation to earthquake physics. Recent discrete models of this failure focused on geometries such as uniaxial tension or anti-plane strain where creation of free surfaces dominates. They are not appropriate for modeling the formation of shearing systems where frictional sliding of material in intimate contact and plastic deformation are important. We present results on a novel approach which introduces damage directly into particle based simulations. When loaded, the model exhibits a period of bursts of spatially correlated damage accumulation followed by a period of catastrophic weakening during which a geometically complex through-going fault network forms, strikingly reminiscent of both laboratory experiments and geophysical observations on the field scale. We will discuss: spatial correlations in damage, evolution of the geometry of the fault system, and the dependence on confining pressures.

1\(^{\text{NSF-DMR-0454947.}}\)
The paper begins with an introduction to the topic of polymer characteristics and their effects on electronic transport in conducting polymers. It mentions the role of nuclear motions in the electron transport and how they are modeled using phonon baths. The authors also include electron-phonon interactions in their consideration.

The authors then describe their experimental setup, which involves the study of doped polymer fibers. They use quantum theory to describe electron transport in mesoscopic systems and assume a conducting state of the material. Conducting polymers, such as polyaniline (PANI), are discussed as the materials of interest.

The results show that PANI-aPAAMPSA, a doped polymer fiber, exhibits better conductivity than PANI-PAAMPSA. These results are corroborated by UV-vis-NIR experiments, where the polaron peak is observed to broaden and red-shift with PANI-aPAAMPSA.

In general, PANI-aPAAMPSA is about twice as conductive as PANI-PAAMPSA of comparable molecular weights. The difference in conductivity is correlated with the polymer acid molecular characteristics.

The paper then shifts to a discussion of silver nanowires, which are synthesized in aqueous solution without surfactant or catalyst. These nanowires are studied using various techniques such as nanoindentation, AFM, and enhanced Raman spectroscopy.

Silver is the metal with the highest electrical and thermal conductivity and has potential applications in electronics. The mechanical behavior of silver nanowires is studied, focusing on their deformation mechanism.

The authors also discuss the aging and plastic deformation in polymer glasses, which is studied using simulations. They investigate the role of intervening adsorbed molecules in nanometer scale mechanical contacts between nominally spherical tips and flat elastic substrates.

Finally, the paper concludes with a discussion of dissipative effects in the electron transport through conducting polymers, where the authors study the effects of stochastic nuclear motions on the electron transport in doped polymer fibers.

The authors acknowledge the financial support from the Department of Energy under grant No.DE-FG02-06ER46293.

Friday, March 9, 2007 8:00AM - 10:48AM
Session X24 DPOLY DMP: Conducting Polymers and Devices
Colorado Convention Center 201

8:00AM X24.00001 Dissipative effects in the electron transport through conducting polymers
NATALYA ZIMBOVSKAYA, University of Puerto Rico at Humacao, GRIGORY ZIMBOVSKIY, Urals State Minig University — Here, we study the effects of stochastic nuclear motions on the electron transport in doped polymer fibers assuming the conducting state of the material. We treat conducting polymers as granular metals and apply the quantum theory of conduction in mesoscopic systems to describe the electron transport between the metallic-like granules. To analyze the effects of nuclear motions we mimic them by the phonon bath, and we include the electron-phonon interactions in consideration. Our results show for some cases the frictional force is proportional to area for bare tips and proportional to load when adsorbed molecules are present.

9:00AM X24.00009 String breaking and the Petersburg Paradox
JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU, LIQUID CRYSTAL INSTITUTE TEAM — The Petersburg Paradox(1) provides a simple paradigm for systems that show critical sensitivity to rare events. The breaking strength of filaments, yarns and strings is determined by the presence of defects. In a given sample, the largest defect determines the stress at which failure occurs, and since the defect distribution is a function of sample size, the breaking strength of strings depends on their length. Analogous to the Petersburg paradox suggests that the breaking strength should vary approximately linearly with the logarithm of the length. We have carried out experiments to measure the breaking strength of samples of polyester sewing thread and of monofilament fishing line ranging in length from 1mm to 1km. We describe our experiments, present the results, and, compare fits of our data to Weibull and mean field failure statistics and the predictions from analogy with the Petersburg Paradox. 1. I. Todhunter, A History of Mathematical Theory of Probability, (Chelsea, New York, 1949)

10:00AM X24.00010 Simulations of aging and plastic deformation in polymer glasses
MYA WARREN, JOERG ROTTLER, University of British Columbia — Experiments on a broad class of amorphous glassy materials show that their mechanical behavior strongly depends on the time since vitrification. The slow relaxation of configurational degrees of freedom, or aging, generally increases the material’s resistance to applied stress. In this study, we investigate the interplay between aging and plastic deformation in a simple model for polymer glasses by means of molecular dynamics simulations. We determine the macroscopic creep compliance for different loading conditions and aging times and find excellent quantitative agreement with experiments: compliance curves can be shifted to form a universal master curve, and the applied stress can reduce the effective age of the glass (molecular rejuvenation). We then measure microscopic, local relaxation times and show that they correlate well with the aging characteristics of the macroscopic creep response. In addition, we explore the evolution of several measures of local order during aging and discuss their role in the mechanical behavior.

10:24AM X24.00111 Deformation mechanism of silver nanowires
MARCEL LUCAS, School of Physics, Georgia Institute of Technology, AUSTIN LEACH, MATT MCDOWELL, KEN GALL, School of Materials Science and Engineering, Georgia Institute of Technology, SIMONA HUNYADI, CATHERINE MURPHY, Department of Chemistry and Biochemistry, University of South Carolina, ELISA RIEDO, School of Physics, Georgia Institute of Technology — Silver is the metal which exhibits the highest electrical and thermal conductivity, and has potential applications in electronics, photonics and catalysis. Silver nanowires could serve as interconnects between electronic circuits, catalysts in chemical reactions, or substrates for surface-enhanced Raman spectroscopy. Understanding how their mechanical properties are affected by their structure (size, cross-section geometry) is essential for their integration in nanodevices. Recently, silver nanowires have been synthesized in aqueous solution without surfactant or catalyst. These nanowires were characterized by Atomic Force Microscopy (AFM) and have a diameter ranging from 20 to 40 nm. Their deformation mechanism was studied by AFM nanoindentation and the results were correlated with atomistic simulations of silver nanowires with a pentagonal cross section.

The authors acknowledge the financial support from the Department of Energy under grant No.DE-FG02-06ER46293.
We measured the laser properties of such microcavities with DOO-PPV polymer as gain medium. Using the spiral microcavity we found unidirectional microcavity configurations; namely a spiral, and a microdisk that contain a linear defect positioned in a specific orientation, have been proposed to overcome this. Such random cavities in thin polymer films by optically characterizing some of the lasing key properties such as size, threshold, and azimuthal window was found. The electrical conductivity of the non-woven fibrous mat and the cast film was measured using the four-point probe method, for different concentrations of Pan.HCSA in the blend. Some possible factors affecting the electrical conductivity of the fibers/films were discussed.

Random lasing action with coherent feedback mechanism was previously attributed to UV-excited oxygen is reflected in a sharp peak in the DOS, whereas in a similar experiment with pentacene oxygen acts as a dopant, and possible defects are found to UV-excited oxygen is reflected in a sharp peak in the DOS. Namely, the ionizing radiation induces a variety of both chemical and structural defects. On the other hand, exposure of rubrene induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. Thus, a profound knowledge of the defect states’ origin is essential. Temperature-dependent space-charge limited current (TD-SCLC) spectroscopy was used as a powerful tool to quantitatively study the density of states (DOS) in high-quality rubrene and pentacene single crystals. In particular, changes of the DOS due to intentionally induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. The optical properties of random cavities are compared with those of a fabricated microdisk having similar size, and the similarities and differences are emphasized.

A group of π-conjugated dendrimers, which are soluble organic molecules consisting of a core group to which branched arms (dendrons) are attached, were synthesized and characterized. These dendrimers have a phenyl core with 3 or 4 arms, i.e., 3 or 4 thiophene dendrons. It has been shown that these dendrimers present a viable alternative to polymers in organic photovoltaic devices with PCBM as the acceptor. We studied electronic structure of these dendrimers by density functional theory and restricted CI singles methods. Quantum mechanical calculations aimed at predicting the optical properties as well as the spatial location of excitons upon photoexcitation were performed. In particular, correlated electron-hole probability diagrams and transition density plots, to be presented here, reveal the nature of excitonic behavior in the dendrimers.

Charge transport in organic molecular crystals is strongly influenced by the density of localized in-gap states (traps). Thus, a profound knowledge of the defect states’ origin is essential. Temperature-dependent space-charge limited current (TD-SCLC) spectroscopy was used as a powerful tool to quantitatively study the density of states (DOS) in high-quality rubrene and pentacene single crystals. In particular, changes of the DOS due to intentionally induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. The optical properties of random cavities are compared with those of a fabricated microdisk having similar size, and the similarities and differences are emphasized.

Semiconducting molecular crystals: Bulk in-gap states modified by structural and chemical defects. Charge transport in organic molecular crystals is strongly influenced by the density of localized in-gap states (traps). Thus, a profound knowledge of the defect states’ origin is essential. Temperature-dependent space-charge limited current (TD-SCLC) spectroscopy was used as a powerful tool to quantitatively study the density of states (DOS) in high-quality rubrene and pentacene single crystals. In particular, changes of the DOS due to intentionally induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. Thus, a profound knowledge of the defect states’ origin is essential. Temperature-dependent space-charge limited current (TD-SCLC) spectroscopy was used as a powerful tool to quantitatively study the density of states (DOS) in high-quality rubrene and pentacene single crystals. In particular, changes of the DOS due to intentionally induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. Thus, a profound knowledge of the defect states’ origin is essential. Temperature-dependent space-charge limited current (TD-SCLC) spectroscopy was used as a powerful tool to quantitatively study the density of states (DOS) in high-quality rubrene and pentacene single crystals. In particular, changes of the DOS due to intentionally induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. Thus, a profound knowledge of the defect states’ origin is essential. Temperature-dependent space-charge limited current (TD-SCLC) spectroscopy was used as a powerful tool to quantitatively study the density of states (DOS) in high-quality rubrene and pentacene single crystals. In particular, changes of the DOS due to intentionally induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. Thus, a profound knowledge of the defect states’ origin is essential. Temperature-dependent space-charge limited current (TD-SCLC) spectroscopy was used as a powerful tool to quantitatively study the density of states (DOS) in high-quality rubrene and pentacene single crystals. In particular, changes of the DOS due to intentionally induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. Thus, a profound knowledge of the defect states’ origin is essential.
10:00AM X24.00011 Transport properties and non-volatile memory application of self-assembled nanoparticle array by microtubules, MEI XUE, K.L. WANG, Device Research Laboratory, Department of Electrical Engineering, University of California, Los Angeles, JING ZHOU, BRUCE DUNN, Department of Material Science & Engineering, University of California, Los Angeles — A method of self-assembly of gold nanoparticles with the diameter of around 1nm is developed by the use of bio species (microtubule) and transport properties of nanoparticle arrays are investigated. Via self-assembly, the attachment sites of gold nanoparticles to the microtubule can be controlled. The density of the gold nanoparticles in our experiments achieved is on the order of 10^9 cm^{-2} and can be extended to as high as 10^{12} cm^{-2}. A transport bi-stability is observed in a sandwich structure of Au/MT + gold nanoparticle array/P-Si substrate. On the basis of detailed analysis of the temperature and electrical field dependences, a band model incorporating electron-tunneling is suggested to explain the observed bi-stability and other transport characteristics. The retention time is also measured to be larger than 10^{7}s. The operation and endurance of this memory device are confirmed. With its simple structure and the compatible fabrication process with conventional MOS, this MT/Au nanoparticle array holds a great potential for memory applications.

10:12AM X24.00012 ABSTRACT WITHDRAWN —

10:24AM X24.00013 Nondestructive Memory Elements Based on Polymeric Langmuir-Blodgett Thin Films, T.J. REECE, S. DUCHARME, Department of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska at Lincoln — Ferroelectric field effect transistors (FeFETs) have attracted much attention recently because of their low power consumption and fast nondestructive readout. Among the ferroelectric thin films used in FET devices, the ferroelectric copolymer of polyvinylidene fluoride, PVDF (C2H2F2), with trifluoroethylene, TFPE (C2H2F2), has distinct advantages, including low dielectric constant, low processing temperature, low cost and compatibility with organic semiconductors. By employing the Langmuir-Blodgett technique, we are able to deposit films as thin as 1.8 nm. We discuss the characterization, modeling and fabrication of metal-ferroelectric-insulator-semiconductor (MFIS) structures incorporating these films.

1This work is supported by the National Science Foundation.

10:36AM X24.00014 Salt-induced phase transitions in charged polymerized membranes, ANGELO CACCIUTO, ERIK LUIJTEN, Department of Materials Science and Engineering and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign — We study the behavior of charged, fully polymerized membranes in the presence of multivalent salt by means of molecular dynamics simulations. At moderate salt concentrations the interplay between the electrostatic interactions and the in-plane elasticity of the membrane gives rise to a novel multi-step folding transition pathway that is qualitatively different from the folding induced by generic attractive interactions at low temperatures. Furthermore, the number of folds in the membrane is greatly reduced when the salt concentration exceeds a critical value, indicating a reentrant transition. Both observations can be viewed as the two-dimensional counterpart of the behavior displayed by flexible linear polyelectrolytes in multivalent salt solutions [1].


Friday, March 9, 2007 8:00AM - 11:00AM — Session X44 DMP: Focus Session: Nanoscale Transport - Molecules III Colorado Convention Center 507

8:00AM X44.00001 Landauer conductance and twisted boundary conditions for Dirac fermions, SHINSEI RYU, Kavli Institute for Theoretical Physics, University of California at Santa Barbara, CHRISTOPHER MUDRY, Paul Scherrer Institute, AKIRA FURUSUKI, RIKEN, ANDREAS LUDWIG, University of California, Santa Barbara — We apply the generating function technique developed by Nazarov to the computation of the density of transmission eigenvalues for a finite graphene sheet in which a two-dimensional freely propagating massless Dirac fermion is localized. By mapping ideal leads associated to the same sample to a conformal invariant boundary condition, we relate the generating function for the density of transmission eigenvalues to the twisted chiral partition functions of fermionic (c=1) and bosonic (c=-1) conformal field theories. We also discuss the scaling behavior of the ac Kubo conductivity and compare its different dc limits with results obtained from the Landauer conductance. Finally, we show that the disorder averaged Einstein conductivity is an analytic function of the disorder strength, with vanishing first-order correction, for a tight-binding model on the honeycomb lattice with weak real-valued and nearest-neighbor random hopping.

8:12AM X44.00002 Electron turbulence in nanoscale junctions, NEIL BUSHONG, University of California, San Diego, JOHN GAMBLE, The College of Wooster, MASSIMILIANO DI VENTRA, University of California, San Diego — Electron transport through a nanos-structure can be characterized in part using concepts from classical fluid dynamics. [1] It is then natural to ask how far the analogy can be taken, and whether the electron liquid can exhibit nonlinear dynamical effects such as turbulence. Here we present a first-principles study using time-dependent current density functional theory of electron transport in nanojunctions which reveals that the electron liquid indeed exhibits behavior quite similar to that of a classical fluid. For example, a transition away from symmetric flow occurs at higher current densities, just as in the classical Navier-Stokes case. We will also discuss the behavior of the velocity correlation tensor in both laminar and turbulent regimes, as well as spontaneous symmetry breaking. Work supported in part by NSF and DOE.


8:24AM X44.00003 Conductance switching and electronic states in polymer nanodevices, NIKOLAI ZHITENEV, Bell Labs., Lucent Technologies, ALEXANDER SIDORENKO, DONALD TENNANT, RAYMOND CIRELLI — Organic materials offer new electronic functionality not available in the inorganic devices. However, the integration of organics within nanoscale electronic circuitry poses new challenges for material physics and chemistry. To rationally control the conducting properties of small devices, the electronic states in organics have to be optimized relative to the Fermi level of metal contacts. We demonstrate a novel approach to create and chemically modify such electronic states in thin polyelectrolyte films. Nanoscale devices fabricated using integrated shadow masks and the polyelectrolyte film grafted to electrodes display reversible switching between conducting and non-conducting states. The conductance is related to the creation and annihilation of the electronic levels in the polymer. The electronic properties and the switching dynamics are broadly tunable by the chemical composition of the polymers. The open design of our nanodevices allows us to perform the chemical conversion targeting primarily carboxyl groups inside the completed junctions. The conduction memory effect is observed in devices with lateral size down to 30 nm.
tied to the two chemical potentials, and the decoherence which cuts off the scaling and leads to effectively classical long-time behavior. In equilibrium problems, the resulting flow equations are used to study the competition between the dephasing-induced formation of independent resonances and the destruction of coherence due to the coupling to the leads. A separation is small or large compared to a dephasing scale defined in terms of the current flowing from one reservoir to another. A nonequilibrium scaling transformation is introduced. An important feature is the presence in the model of a new coupling, essentially the decoherence rate, which acquires an additive renormalization similar to that of the energy.

The normalized linear conductance as a function of $T/T_K$ differs from the scaling function expected for the spin-1/2 Kondo problem, which is described by the $H_S(1)$ intracage vibrational mode of C$_{60}$. Changes in electrode spacing can tune the energy and amplitude of these signals.

Present address: California Institute of Technology

9:12AM X44.00005 Tuning the Kondo effect with a mechanically controllable break junction

The work was supported by NYSTAR.

9:36AM X44.00007 Interference Effects in Nanoscale Electron-Phonon Transport

1Perform in collaboration with B. K. Foster, R. G. Harris, L. S. Mattos, and C. R. Moon. This work was supported by DOE, NSF, and ONR.

2Department of Applied Physics

3Department of Physics

10:00AM X44.00009 Coulomb gas scaling of the non-equilibrium spin-boson model

1Acknowledgements: This work was supported by NSF-DMF 0431350
10:12AM X44.00010 Numerical Estimation of Keldysh-Countour Path Integrals for Nonequilibrium Problems\textsuperscript{1}, ANDREW MILLIS, Columbia University, PHILIPP WERNER — We propose an idea for simulating the dynamics of open (coupled to reservoirs) systems in nonequilibrium steady state and present preliminary numerical results for the nonequilibrium spin boson and Anderson models. The method builds on the observation (Phys. Rev. Lett. 94 076404) that out of equilibrium the Keldysh time evolution operator exhibits an exponential-time decay, and uses the stochastic hybridization expansion techniques of Phys. Rev. Lett. 97, 076404.

\textsuperscript{1}Supported by NSF-DMR-04031350

10:24AM X44.00011 Full Counting Statistics for a Single-Electron Transistor: Nonequilibrium Effects at Intermediate Conductance, YASUHIRO UTSUMI, DIMITRI GOLUBEV, GERD SCHÖN, Institut für Theoretische Festkörperphysik, Universität Karlsruhe — We calculate the probability distribution of current for a single-electron transistor (SET) with intermediate strength conductance where quantum fluctuations of the charge play a dominant role. The calculations are based on the multichannel anisotropic Kondo model in the Majorana representation and the fermionic Keldysh generating functional. The effects of quantum fluctuations are taken into account by the summation of a certain subclass of diagrams, which corresponds to the leading logarithmic approximation in the sense that the result is consistent with the RG analysis. We have shown that in non-equilibrium situations quantum fluctuations of the charge induce lifetime broadening for the charge states of the central island. Consequences which can be detected in experiments include a suppression of the probability currents larger than the average value. Y. Utsumi, D. Golubev, G. Schoen; PRL. 96, 086803 (2006)

10:36AM X44.00012 Vibronic coupling effect on the electron transport through molecules, MASARU TSUKADA, Waseda University, KUNIHIRO MITSUTAKE, Canon Research Center, Canon Inc. — Electron transport through molecular bridges or molecular layers connected to nano-electrodes is determined by the combination of coherent and dissipative processes, controlled by the electron-vibron coupling, transfer integrals between the molecular orbitals, applied electric field and temperature. We propose a novel theoretical approach, which combines ab initio molecular orbital method with analytical many-boson model. As a case study, the long chain model of the thiophene oligomer is solved by a variation approach. Mixed states of moderately extended molecular orbital states mediated and localized by dress of vibron cloud are found as eigen-states. All the excited states accompanied by multiple quanta of vibration can be solved, and the overall carrier transport properties including the conductance, mobility, dissipation spectra are analyzed by solving the master equation with the transition rates estimated by the golden rule. We clarify obtained in a uniform systematic way, how the transport mode changes from a dominantly coherent transport to the dissipative hopping transport.

10:48AM X44.00013 Quantum open systems approach to single-molecule devices, YONGQIANG XUE, WILLIAM KENNERLY, University of California at Albany-SUNY — Experimental advances in electrically and optically probing individual molecules have provided new insights into the behavior of single quantum objects and their interaction with the nanoenvironments without requiring ensemble average. Single-molecule devices are open quantum systems whose dynamics are intrinsically stochastic and are subject to dissipation and decoherence through system-environment correlation. New concepts and computational techniques may be needed to unravel the rich physics underlying single-molecule measurements. In this talk, we discuss our efforts in developing quantum open systems theory of single-molecule electronics and optics, building on concepts and techniques from quantum optics and quantum measurement.

Friday, March 9, 2007 11:15AM - 2:15PM —
Session Y9 DMP: Superconductivity: Josephson Junctions, Proximity Effect & Squids II

11:15AM Y9.00001 Microwave characterization of Josephson junctions arrays for Coulomb blockade, VLADIMIR MANUCHARYAN, MICHAEL METCALFE, R. VIJAY, ETIENNE BOAKNIN, MICHEL DEVORET, Yale Applied Physics — Coulomb Blockade of a single Josephson junction leads to oscillations in time of the voltage across the junction when a DC electrical current is applied. Because the frequency $f$ of these so-called Bloch oscillations is related to the current $I$ only through the charge $2e$ of a Cooper pair, $f = 1/2e$, the phenomenon can be utilized to build a primary standard of electrical current. However, to reach the regime of Coulomb blockade, the current must be applied to the junction through the leads with electromagnetic impedance exceeding the quantum of resistance for Cooper pairs (6.5 kΩ) at frequencies $\omega \approx h/E_c$, $E_c$ being the charging energy of the junction. For typical parameters $\omega_c$ lies in the microwave domain, where electromagnetic impedances tend to be of the order of the free space impedance ($377 \Omega$). This fundamental mismatch in the impedance turns the realization of a current standard based on Bloch oscillations into a very challenging problem. Our proposal is to use kinetic impedance of a superconductor, namely, the Josephson inductance. We have fabricated arrays of large Josephson junctions which are superconducting at DC and characterized them at microwave frequencies. Our results indicate that these arrays are capable of beating the impedance quantum and we are setting up an experiment on electrical current metrology.

11:27AM Y9.00002 Low-frequency Critical Current Fluctuation Measurements in Nb/AlOx/Nb Junctions\textsuperscript{1}, SHAWN POTTORF, VIJAY PATEL, J. E. LUKENS, Stony Brook University — We have measured the low frequency critical current noise in Nb/AlOx/Nb Josephson junctions used for qubits in quantum computation circuits. Low frequency current noise measurements were made using a bridge circuit with a SQUID null detector. The current noise spectra density showed a $1/f$ component at low frequencies for both an unshunted junction biased near $6 \mu V$ and a shunted junction biased near $7 \mu V$. In both cases this corresponded to critical current fluctuations with a spectral density at 1 Hz of $2.2 \times 10^{-25} \text{A}^2/\text{Hz}$. Our measured value of critical current fluctuations is roughly two orders of magnitude less than the average of various technologies reported by Van Harlingen et al. (2004).

\textsuperscript{1}This work is supported in part by AFOSR and NSA through a DURINT program and by NSF.

11:39AM Y9.00003 Microscopic Model of $1/f$ Noise in Josephson Junctions, MAGDALENA CONSTANTIN, CLARE YU, Department of Physics and Astronomy, University of California, Irvine, California 92697, JOHN MARTINIS, Physics Department, University of California, Santa Barbara, California 93106 — We present a simple microscopic model to show how fluctuating two-level systems in the Josephson junction tunnel barrier can modify the potential energy of the barrier and produce critical current noise spectra as well as charge noise. We find $1/f$ critical current and charge noise at low frequencies. Our values are in good quantitative agreement with recent experimental measurements of noise in Al/AlOx/Al Josephson junctions. We also investigate the sensitivity of the critical current noise on the nonuniformity of the tunnel barrier.
11:51AM Y9.00004 High-frequency spectroscopy and emission properties of a single-Cooper pair transistor, PIERRE-MARIE BILLANCEON, Laboratoire de Physique des Solides, associé au CNRS, Bât. 510 Université Paris-Sud, FRÉDÉRIC PIERRE, Laboratoire de Photonique et Nanostructures, associé au CNRS, Bât. 510 Université Paris-Sud — We have characterized the high-frequency properties of a single-Cooper pair transistor (SCPT), by a capacitive coupling with a Josephson junction. We have alternately used the Josephson junction (JJ) as a high-frequency generator by using the AC Josephson effect, and as a high-frequency detector by using the photo-assisted tunneling current. We have been able to induce transitions between the first energy levels of a SCPT, thanks to the high-energy photons emitted by the AC Josephson effect. This allowed us to perform a high-frequency spectroscopy of a SCPT (10-200 GHz). Moreover, as the emitted photons can have an frequency higher than the superconducting gap of the island, we can not only induce the transfer of Cooper pairs, but also quasiparticles, allowing us to control the poisoning of the SCPT. Then, we used the Squid geometry of the Josephson junction in order to tune its Josephson energy to zero, and use it as a high-frequency detector. We have been able to detect different kinds of high-frequency emission process associated with the coherent transfer of Cooper pairs through the SCPT (AC Josephson effect), and the resonant transfer of Cooper pairs, already characterized in transport measurements by Joyez et al.

12:03PM Y9.00005 Using a High-Q Josephson Resonator as a Non-Dissipative RF-SQUID, J.A. STRONG, NIST, Boulder, K.D. OSBORN, A.J. SIROIS, R.W. SIMMONDS — Superconducting Quantum Interference Devices (SQUIDs) have been used for years to measure small magnetic fields. Such devices measure the DC voltage across a Josephson junction as a function of magnetic flux. It is well known, however, that a voltage biased Josephson junction radiates energy. This is problematic for many superconducting quantum device applications including readout methods for superconducting quantum bits and SET’s. Here, we examine a newly developed Josephson junction resonator as a new breed of SQUID, wherein the resonator’s resonant frequency (instead of the junction’s voltage) is measured as a function of magnetic flux. In this way, the Josephson junction is kept perpetually in the super-current state, with zero DC voltage and therefore no Josephson radiation. We examine issues of sensitivity, noise, and read-out speed.

12:15PM Y9.00006 Cooper-pair Tunneling in a High Impedance Environment, M. A. CASTELLANOS-BELTRAN, K. W. LEHNERT, JILA, NIST and the Department of Physics, University of Colorado, Boulder, Colorado 80309-0440, USA. — Coulomb blockade of current and coherent oscillations in the voltage across a small tunnel junction can only be observed if the junction is embedded to being blockade-like as the microwave power level increases, and the zero-bias resistance $R_Q = 6.5 \, k\Omega$ at all relevant frequencies (DC - 20 GHz). We will show results from two different experiments that characterize the impedance of one-dimensional Josephson junction arrays. First, by using the array to bias a SQUID made from small area junctions, we show the behavior of this system can only be explained if the array creates an environment with an impedance several times $R_Q$. Second, we measure the speed at which microwave signals propagate through co-planar waveguides whose inner conductors are formed from an array of Josephson junctions. We find that these waveguides behave as LC transmission lines with wave impedances of several $k\Omega$ and wave speeds less than 1% of the speed of light in free space.

12:27PM Y9.00007 Adiabatic Perturbing a Bloch Transistor by Microwave Irradiation: Inversion of Coulomb Oscillation, WATSON KUO, SAXON LIOU, Y.W. SUEN, Department of Physics, National Chung Hsing University, Taichung 402, Taiwan, W.H. HSIEH, C.S. WU, C.D. CHEN, Institute of Physics, Academia Sinica, Nankang 105, Taiwan — We experimentally studied the switching current and DC current-voltage (IV) characteristics of a Bloch transistor irradiated with microwaves of frequency from several GHz up to 18GHz. The photon energy is well below the level spacing of the two-level quantum states so that the Bloch transistor is perturbed in the adiabatic regime. Phase-charge duality in a Josephson junction is clearly seen in the switching current distribution as a function of gate voltage. The reduction of switching current due to photon excitation is significant when the phase fluctuation is small. In particular, an inversion of Coulomb oscillation of switching current is observed at a higher microwave power level. When the microwave frequency is below 7GHz, the IV characteristics of the Bloch transistor evolve from being superconductor-like to being blockade-like as the microwave power level increases, and the zero-bias resistance $R_0$ shows a Coulomb oscillation accordingly: when $R_0$ is maximal, the switching current is also maximal, opposite to that without microwave irradiation. As the microwave power level increases further, Shapiro steps in IV characteristics are observed. The step height can be analyzed using a model for an ac voltage source applied to a single Josephson junction.

12:39PM Y9.00008 Superconductor-normal metal contact conductance of a graph node, VLADIMIR LUKIC, ELISABETH NICOL, University of Guelph — We study the conductance of a superconductor-normal metal (SN) contact with the topology of a graph node. We derive the extension of the Blonder-Tinkham-Klapwijk (BTK) equations using the boundary conditions for a wavefunction at a graph node, and show that in the appropriate limit they reduce to the standard BTK formula for an SN contact. Qualitatively new conductance features arise from crossed Andreev reflection and interference of partially reflected waves from different graph legs, and we demonstrate their importance by using the Landauer method to rederive the formula for conductance. The relevance of these effects to experiment will be discussed.

1:03PM Y9.00009 Singular length dependence of critical current in superconductor/normal-metal/superconductor bridges, ALEX LEVCHENKO, ALEX KAMENEV, LEONID GLAZMAN, University of Minnesota — We examine the dependence of the critical Josephson current on the length $L$ of the normal bridge $N$ between two bulk superconductors. This dependence turns out to be nonanalytic at small $L$. The nonanalyticity originates from the contribution of extended quasiparticle states with energies well above the superconducting gap. This should be contrasted with the more familiar contribution to the Josephson current coming from Andreev bound states localized in the normal region at energies below the gap. We also have preliminary results on the ac Josephson effect above the critical temperature $T_c$ where we have studied the influence of the superconducting fluctuations on the current noise. It turns out that the current noise acquires singular in $T - T_c$ correction, which is peaked at the Josephson frequency. This correction originates from the fluctuating ac Josephson current.

1:03PM Y9.00010 Interaction of breathers with moving vortices in a Josephson junction ladder, DEVIN EDWARDS, KEN SEGALL, Colgate University, JUAN MAZO, University of Zaragoza — Josephson junction arrays offer an important method to experimentally study nonlinear dynamics. We have studied Nb-AIOx-Nb Josephson junction ladder arrays with 24 periods which support two distinct nonlinear modes. The first is a discrete breather, which is a spatially localized excitation that does not propagate through the ladder. The second is a propagating two pi phase shift, or moving vortex. Both modes have been observed independently in our arrays. Predictions have been made regarding the dynamics of the interactions of these two modes, but these have not been verified experimentally. One such prediction is that under some conditions the breather will pin the propagating vortices and prevent them from passing beyond the breather. We will present theoretical simulations and recent experiments attempting to observe their interaction.
1:15PM Y9.00011 Fluxon ratchet dynamics in a Josephson junction array

KENNETH SEGALL, ADAM DIOGUARDI, NIKHIL FERNANDES, USHNIH RAY, Colgate University, JUAN MAZO, FERNANDO NARANJO, University of Zaragoza — We present theoretical and experimental work on the ratchet dynamics of fluxons in an array of Josephson junctions. Fluxons trapped in a parallel array of Josephson junctions upon cooldown experience a potential determined by the junction critical currents and the cell inductances. By varying these quantities in an asymmetric way, the potential can be made ratchet. We probe the dynamics of the fluxon with switching current measurements, which allow determination of the transition rate of the fluxon from its pinned state to a running state. We find two temperature regimes, both experimentally and in simulations. At low temperatures, the fluxon behaves like a single particle and undergoes thermal activation. At intermediate temperatures, the fluxon undergoes diffusion for several periods and then jumps to the running state. The dynamics in this region cannot be explained with a single particle picture. We have observed two temperature-dependent crossovers in the direction of transport in this temperature region. We present temperature-dependent measurements, comparisons with simulation, and possible interpretations of the crossovers.

1:27PM Y9.00012 Manipulation of half-integer flux quanta

C. J. M. VERWIJ, ARIANDO, J. A. BOSCHKER, H. HILGENKAMP, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente — Because of the different pairing symmetry in high-Tc cuprates (d-wave) and low-Tc superconductors (s-wave) it is possible to realize hybrid superconducting rings with a built-in π-phase shift. These rings have a twofold degenerate groundstate characterized by spontaneously generated circulating currents corresponding to a half flux quantum. We have realized such rings by connecting the cuprate YBa2Cu3O7−δ to the low-Tc superconductor Nb via ramp-type Josephson junctions. We present the integration of π-rings in a superconducting quantum electronics device, a toggle flip-flop, in which the fractional flux polarity is toggled by applying single flux quantum pulses. We will also present experiments in which the half flux quanta at the discontinuities of 0−π Josephson corner junctions are manipulated.

1:39PM Y9.00013 Vortex flow characteristics of Bi2Sr2CaCu2O8+δ Long Intrinsic Josephson Junctions

KAZUO KADOWAKI, KOHEI KAWAMATA, YUIMARU KUBO, KAZUKI FUKUI, TAKASHI YAMAMOTO, ITSUHIRO KAKEYA, Institute of Materials Science, University of Tsukuba — Intrinsic Josephson junction characteristics in Bi2Sr2CaCu2O8+δ, where the junction length L is much longer than the Josephson length λJ=γE0/2π, have been studied from view point of Josephson vortex dynamics, since they are expected to be released from the strong geometrical constraint, which confines Josephson vortices into a square box, and as a result they are free to move in the two dimensional channels. We fabricated such long junctions with L=20-40 μm and have measured c-axis transport characteristics. We have found that Josephson flow resistance RF suddenly suppressed at the intermediate field region of 1-2 T, then begins to reappear gradually as field is increased. The sharp lock-in transition as a function of angle appearing below it where the periodic oscillation of RF is seen, becomes immediately broad and a round peak above it, where the periodic oscillation of RF is no longer observable. It seems that the transition field becomes lower as L is increased so that in short junctions it cannot be observed in a field region up to 6 T.

1:51PM Y9.00014 Optimization of HighTc Josephson nanojunctions by Monte Carlo simulations

M. SIRENA, N. BERGJAL, J. LESUEUR, ESPCI - LPQ, 75231 Paris, France, G. FAINI, LPN-CNRS, 91460 Marcoussis, France, R. BERNARD, J. BRIATICO, D. CRETE, UMR CNRS/THALES, 91120 Palaiseau, France — The fabrication of YBCO JJ by ion damage is the best method that allows closed packed JJ series within the nanoscale and that could operate at high temperature. However, the strong variation of the JJ’s critical current with temperature (T) and the increase of dispersion for high irradiation dose are still important issues for several applications. Reproducible HTc JJ have been produced combining electron beam lithography and ion beam irradiation, whose characteristics can be adjusted on a wide range of T. To further improve the homogeneity of planar JJ and optimize their behaviour, we have studied its lateral ion damage distribution (LDD) for different ions and incident energies using Monte Carlo simulations. The LDD was used to calculate the transition temperature (Tc) of the irradiated zone and its resistance as a function of T. Dispersion in the irradiation mask’s size was introduced as the source of the JJ’s in-homogeneity. The simulations results reproduce quite well the observed dispersion of the irradiated JJ. A linear behaviour of the JJ’s Tc dispersion with basically the LDD width was found, independent of the incident ions mass, its energy, the films thickness, etc. By choosing the appropriate parameters is possible to increase the JJ homogeneity, reducing the LDD width.

2:03PM Y9.00015 Fiske and size-independent resonances in /J−V/ characteristics of micron-sized Bi2Sr2CaCu2O8+δ single crystals

ITSUHIRO KAKEYA, YUIMARU KUBO, MASASHI KOHRI, KAZUKI FUKUI, KOHEI KAWAMATA, TAKASHI YAMAMOTO, KAZUO KADOWAKI, Institute of Material Science, University of Tsukuba, 1-1-1, Ten-nodai, Tsukuba, 3058573, Japan — We have investigated the c-axis transport properties of micron-size Bi2Sr2CaCu2O8+δ (Bi2212) single crystals fabricated by the focused ion beam method under magnetic field parallel to the ab-plane. It was found that periodic current steps in current-voltage (J−V) characteristics, whose features are similar to the Fiske step known in a single Josephson junction. We also found another current step with non-oscillating field dependence in low voltage region. Since the voltage of this step does not depend on the sample size unlike the Fiske step, it is considered that the step is attributed to an intrinsic phase excitation of Bi2212.
Ultrafast hole-spin dynamics in bulk GaAs, HANS CHRISTIAN SCHNEIDER, MICHAEL KRAUSS, Physics Dept., Kaiserslaunten University — This talk presents theoretical results on hole-spin dynamics in bulk GaAs after optical excitation. The coupled dynamics of spin and orbital angular momentum is determined by solving dynamical Boltzmann equations for carrier-carrier scattering, which include the effect of spin-orbit coupling on the level of a 4-band Luttinger Hamiltonian. Hole-spin relaxation takes place in two stages. In the first regime, on a timescale of a few hundred femtoseconds, pure momentum scattering dominates the dynamics and the anisotropic contributions to the orbital angular momentum, which are created by the optical excitation, are evened out. In the second regime, on a timescale of a few picoseconds, energy relaxation dominates. The hole-spin dynamics can be approximated by a different relaxation time for each of the two regimes. The fast spin relaxation-time in the first regime is in agreement with experimental results for heavy-hole spin relaxation.

This work was supported by DARPA SpinS program and the Dynasty Foundation (Russia)
12:51PM Y12.00009 Evolution of coherently controlled charge and spin currents injected by optical pulses.1, R. ABRAROV, A. NAJMAIE, E. YA. SHERMAN, J. E. SIPE, Department of Physics and Institute for Optical Sciences, University of Toronto, St. George Street 60, Toronto, Ontario, Canada, DEPARTMENT OF PHYSICS AND INSTITUTE FOR OPTICAL SCIENCES, UNIVERSITY OF TORONTO, ST. GEORGE STREET COLLABORATION — We consider dynamics of coherently controlled currents injected by short (100 fs) optical pulses with frequencies \( \omega \) and \( 2\omega \) in multiple GaAs/AlGaAs quantum wells. Our approach is based on the series expansion of the carrier and current densities in an appropriate set of basis functions. The role of space-charge effects (long-range Coulomb interaction between electrons and holes) and current-conserving and non-conserving collisions of the carriers on the dynamics of the quantities observable in pump-and-probe experiments is investigated. We show that under certain conditions, dependent on the relaxations rates and the band structure effects, displacement of electrons and holes from the initial positions can be finite even on a long time scale of the order of few picoseconds. Due to the skew scattering arising during electron-hole collisions, injected charge (spin) currents drive the spin (charge) currents which can be observed experimentally.

1This work was supported by DARPA SpinS program

1:03PM Y12.00010 Bias-Dependent Electron Spin Lifetimes in n-Type GaAs and the Role of Donor Impact Ionization M. FURIS, University of Vermont, Burlington, Vermont, D.L. SMITH, S.A. CROOKER, Los Alamos National Laboratory, Los Alamos, NM, J.L. RENO, Sandia National Laboratories, Albuquerque, New Mexico — We present a study of electron spin lifetimes \( \tau \) of Donor Impact Ionization, M. FURIS, University of Vermont, Burlington, Vermont, D.L. SMITH, S.A. CROOKER, Los Alamos National Laboratory, Los Alamos, NM, J.L. RENO, Sandia National Laboratories, Albuquerque, New Mexico — We present a study of electron spin lifetimes \( \tau \) on a long time scale of the order of few picoseconds. Due to the skew scattering arising during electron-hole collisions, injected charge (spin) currents drive the spin (charge) currents which can be observed experimentally.

1:15PM Y12.00011 Spin precession and spin relaxation in semiconductors , DIMITRIE CULCER, ROLAND WINKLER, Advanced Photon Source, Argonne National Laboratory, Argonne IL 60439, and Northern Illinois University, De Kalb IL 60115 — In order to achieve a lasting spin polarization a proper understanding of the mechanisms leading to spin polarization decay is critical. We present a general theory for spin polarization decay due to the interplay of spin precession and momentum scattering that is applicable to both spin-1/2 electrons and spin-3/2 holes and that allows us to identify and characterize a wide range of qualitatively different regimes [1]. The spin polarization of ballistic carriers is reduced by spin dephasing, which is characterized by a non-exponential time dependence and results in an incomplete decay of the spin polarization. For weak momentum scattering or fast spin precession, the spin relaxation time is proportional to the momentum relaxation time. For strong momentum scattering and slow spin precession we recover the D'yakonov-Perel result that the spin relaxation time is inversely proportional to the momentum relaxation time. [1] D. Culcer and R. Winkler, cond-mat/0610779.

1:27PM Y12.00012 Spin relaxation of electrons in bulk CdTe DANIEL SPRINZL, PETRA NAHALKOVA, JAN KUNC, PETR MALY, PETR HORODÝŠKY, ROMAN GRILL, EDUARD BELAS, JAN FRANC, PETR NEMEC, Faculty of Mathematics and Physics, Charles University in Prague — We report on the measurements of the spin relaxation time \( T_1 \) of photo-excited electrons in bulk CdTe. The carrier dynamics were investigated by transient absorption experiments using 80 fs circularly polarized laser pulses at sample temperatures from 20 to 300 K. We studied both p and n type doped CdTe samples, which were prepared in the form of thin platelets from the crystals grown by the modified Bridgman method. The obtained results are compared with the spin relaxation times reported for other semiconductors with the same crystal structure (e.g., GaAs [1]). Finally, the relative contributions of the D'yakonov-Perel, Elliott-Yafet, Bir-Aronov-Pikus, and other mechanisms to the measured spin relaxation times in CdTe are discussed. This work was supported by the Grant Agency of the Czech Republic (grant 202/03/H003), by the Ministry of Education of the Czech Republic in the framework of the research centre LC510 and the research plan MSM 0021620834. [1] J. M. Kikkawa and D. D. Awschalom, Phys. Rev. Lett. 80, 4313 (1998).

1:39PM Y12.00013 Suppression of nuclear polarization in photon-irradiated GaAs M.R. FITZSIMONS, B.J. KIRBY, F. TROUW, LANL. A. CROWELL, C. ADELMANN, S.D. FLEXNER, C.J. PALMSTROM, M. ERICKSON, UMN, J.A. BORCHERS, C.F. MAJKRZAK, W. CHEN, T.R. GENTILE, NIST, R. PYNN, UI — We measured the spin dependence of polarized neutron beams reflected by a GaAs sample at 20 K in a magnetic field of 250 Oe applied along the sample's surface normal. Neutron data were acquired with left and right circularly polarized light (0.25 W/cm\(^2\) and 808 nm) illuminating the sample. These conditions yielded nuclear polarization in the same sample (before and after the neutron experiment) of several percent as evidenced by a shift of a peak in the optical Hanle curve. The neutron data exhibit a correlation with light polarization and thus nuclear polarization. Quantitative analysis of the spin dependence of the polarized neutron reflectivities indicates nuclei within 50 nm of the sample’s surface are not polarized, and then nuclear polarization increases to a small value in the bulk. We attribute suppression of nuclear polarization near the sample’s surface to the electric field in the depletion layer that inhibits binding of spin polarized carriers to donor sites and to the electric field gradient at the nuclei (induced by the electric field in the depletion layer) that depolarizes nuclei with quadrupole moments such as Ga and As.

1:51PM Y12.00014 ABSTRACT WITHDRAWN —

2:03PM Y12.00015 Electric field dependence of the electron g-factor for a Si donor in bulk GaAs A. DE, CRAIG E. PYOR, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa — Modulation of the electron g-factor by an applied electric field may be used to coherently manipulate spins for quantum information processing. We present numerical calculations of the electric field dependence of the g-factor of an electron bound to a silicon donor in bulk GaAs. The calculations were carried out using 8-band k\( \cdot \)p theory in the envelope function approximation, which is implemented using finite differences on a real-space grid. The binding energy of the Si impurity in GaAs was fit to experimental data by adding a central cell correction to the donor site. Electrically modulating the impurity’s g-factor is possible as the electric field modifies the binding energy for the Si donor. In our calculations, it is seen that the variation in \( g \) is nearly quadratic as a function of electric field (up to 0.2 mV/nm) and for \( E = 0 \), \( \frac{d^2g}{dE^2} = 1.2 \text{ (mV/nm)}^{-2} \). The largest variation in \( g \) is obtained when the applied magnetic field and electric fields are in the same direction. The proposed scheme provides a realizable alternative to quantum information processing using quantum dots.

Friday, March 9, 2007 11:15AM - 2:15PM —
Session Y13 DMP GMAG: Focus Session: Charge/Orbital Order in Complex Oxides Colorado Convention Center Korbel 4C
11:15AM Y13.00001 Commensurate and incommensurate charge order in Fe$_2$OBO$_3$. MANUEL ANGST, Oak Ridge National Laboratory, Oak Ridge TN 37831, RAPHAEL HERMANN, FZ Juelich, 52425 Juelich, Germany, JONG-WOO KIM, Ames Laboratory, Ames IA 50011, PETER KAHLIFAH, U Massachusetts, Amherst MA 01003, BRIAN C. SALES, DAVID G. MANDRUS, Oak Ridge National Laboratory, Oak Ridge TN 37831 — Charge order CO in the form of a Wigner crystal had been proposed by Attfield et al. [Nature 396, 655 (1998)] based on measurements, particularly Möbbauer spectroscopy, on polycrystalline Fe$_2$OBO$_3$, but no superstructure due to the CO had been detected. We have grown the first single crystals of pure Fe$_2$OBO$_3$, and resistivity and thermal analysis indicate not one, but two transitions associated with CO. To elucidate the nature of these two transitions a synchrotron study was performed. At low $T$ a superstructure corresponding to a doubling of the $a$ axis was observed for the first time. The phase between the two phase transitions, in contrast, exhibits an incommensurate modulation with propagation vector $(\frac{1}{2}, 0, \tau)$, $\tau$ increasing with $T$ towards $\frac{1}{2}$. Resonances in the energy-dependence of the scattered intensity around the Fe $K$ edge suggest that the modulations in both phases are indeed associated with CO.

11:27AM Y13.00002 Optical study of Cubr$_2$S$_4$ and MgTi$_2$O$_4$: experimental support for orbital-Peierls transitions. NAN LIN WANG, JUN ZHOU, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, PR China, GUANGHAN CAO, Department of Physics, Zhejiang University, JING SHI, Department of Physics, Wuhan University — In metals with low-dimensional electronic structure, Fermi surface instability can drive a system into a symmetry-breaking insulating state. However, such instability is not expected to develop in a three-dimensional (3D) system. Recently two types of highly exotic orderings were discovered by Radaelli et al. in two spinel compounds: an octamer ordering in CuIr$_2$S$_4$ and a helical ordering in MgTi$_2$O$_4$. In both cases, sharp metal-insulator transitions (MIT) and spin-dimerizations associated with the structural distortions occur simultaneously. It was suggested that the orbital degree of freedom plays a key role in such transition: the ordering of the orbitals makes the first single crystals of pure Fe$_2$OBO$_3$, but no superstructure due to the CO had been detected. We have grown the first single crystals of pure Fe$_2$OBO$_3$, and resistivity and thermal analysis indicate not one, but two transitions associated with CO. To elucidate the nature of these two transitions a synchrotron study was performed. At low $T$ a superstructure corresponding to a doubling of the $a$ axis was observed for the first time. The phase between the two phase transitions, in contrast, exhibits an incommensurate modulation with propagation vector $(\frac{1}{2}, 0, \tau)$, $\tau$ increasing with $T$ towards $\frac{1}{2}$. Resonances in the energy-dependence of the scattered intensity around the Fe $K$ edge suggest that the modulations in both phases are indeed associated with CO.

11:39AM Y13.00003 Orbital ordering in spinel AV$_2$O$_4$ (A=Mn,Fe). T. KATSUFUJI, T. SUZUKI, M. KATSUMURA, H. TAKEI, Dept. of Physics, Waseda University, K. TANIGUCHI, T. ARIMA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University — In spinel vanadates, AV$_2$O$_4$ (A=ivalent ion), there is an orbital degree of freedom in the V$^{3+}$ ion, which contains two d electrons in the triply degenerate $t_g$ orbital. We measured the x-ray diffraction of the single crystal of MnV$_2$O$_4$, which exhibits simultaneous ferrimagnetic and a structural phase transition at 57 K, and found that a diamond-glide symmetry is broken in the ferrimagnetic tetragonal phase in this compound, indicating the antiferro-type ordering of the $t_g$ orbitals. This orbital ordering can be explained by the enhancement of the antiferro-orbital interaction caused by the ferromagnetic alignment of the V spins in the ferrimagnetic phase. We also measured the x-ray diffraction of the FeV$_2$O$_4$ single crystal, and found that a different type of orbital ordering from that of MnV$_2$O$_4$ occurs in this compound.

11:51AM Y13.00004 Magnetic fluctuations and orbital orderings in ferrimagnetic spinels. JAE-HO CHUNG, NIST Center for Neutron Research and University of Maryland, JUNG HWA KIM, SEUNG-HUN LEE, University of Virginia, TAKU S. SATO, University of Tokyo, TAKURO KATSUFUJI, Waseda University — We report our inelastic neutron scattering studies of two related spinels, AB$_2$O$_4$ (A=Mn, B=Mn and V), with $e_d$ and $t_g$ orbital degeneracy, respectively. Both systems undergo noncollinear triangular ferrimagnetic orderings at low temperatures, where the lattice symmetries are tetragonal. Characteristics of the phase transitions, however, are different. In the case of Mn$_3$O$_4$, the tetragonal distortion with $c > a$ exists below $T = 1443$ K, and upon cooling a noncollinear ferrimagnetic ordering occurs at 42 K, followed by two more magnetic transitions into commensurate ($40$ K) and commensurate cell doublings ($34$ K). Those magnetic phases exhibit magnetocapacitance. In the case of MnV$_2$O$_4$, on the other hand, a collinear ferrimagnetic ordering occurs at 65 K, followed by the tetragonal distortion with $c < a$ and a noncollinear ordering at 58 K. Our single crystal inelastic neutron scattering data show magnetic excitations up to 20 meV for Mn$_3$O$_4$ and up to 40 meV for MnV$_2$O$_4$. We have performed linear spin wave calculations to obtain their effective Hamiltonians by comparing the calculated dispersions of spin waves to the observed ones. The implications of the spin Hamiltonians to their orbital states, and the polarization of spin waves will be discussed.


12:39PM Y13.00006 Orbital ordering in striped phases of La$_{1-x}$Ca$_x$MnO$_3$: GGA+U versus GGA results. NADIA BINGGELI, ICTP and INFN-CNR DEMOCRITOS National Simulation Center, Trieste, Italy, GIANCARLO TRIMARCHI, National Renewable Energy Laboratory — We have investigated the orbital ordering in La$_{1-x}$Ca$_x$MnO$_3$, with $x=2/3$ and 1/2, within the generalized gradient approximation (GGA) of density functional theory and within the GGA plus onsite Coulomb interaction (GGA+U) approach. The calculations were performed using the pseudopotential plane-wave scheme and include structural relaxation. In the half-doped case, similar results are obtained for the orbital and atomic structure within the two approaches, with structural properties consistent with experiment. For the two-thirds-doped system, instead, the results differ between the two approaches. Only the GGA+U yields an insulating striped phase with structural properties in agreement with experiment. Our results show the importance of the cooperative effects of the Jahn-Teller distortion, strain modulation, and electronic localization in stabilizing the orbital-ordered striped phases, and provide new insight into the atomic-scale structure of the orbital order in La$_{1/3}$Ca$_{2/3}$MnO$_3$.

12:51PM Y13.00007 Direct evidence of charge inhomogeneity during the commensurate-incommensurate phase transition in charge ordered La$_{1-x}$Ca$_x$MnO$_3$. J. TAO, M. VARELA, S. J. PENNYCOOK, Oak Ridge National Lab, J. M. ZUO, UIUC — Commensurate-incommensurate (C-IC) phase transitions occurring in charge ordered (CO) manganites have been measured extensively by neutron scattering, x-ray diffraction and electron diffraction. However, these measurements only provide an average picture of the CO transition. Direct observations at the nano-scale are lacking, and the exact mechanism underlying the CO phase transitions remains unknown. Here, we report our in-situ electron microscopic studies of the CO C-IC phase transition in La$_{0.2}$Ca$_{0.8}$MnO$_3$. Scanning an electron probe about 1.7 nm in size over the sample, the local CO structures are recorded in the electron nano-diffraction patterns and the super-reflections associated with the CO phase are used to study the local effective doping. The mapping of the CO phase clearly shows inhomogeneous patterns of phase separation during the phase transition. The C-IC phase transition is interpreted by the change of the distribution of electrons/holes in La$_{1-x}$Ca$_x$MnO$_3$.

1This research was sponsored by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC.
Competing Ferromagnetic and Charge-Ordered States in Realistic Models for Manganites: the Origin of the CMR Effect, CENGIZ SEN, National High Magnetic Field Lab and Florida State University, Tallahassee, FL, GONZALO ALVAREZ, Oak Ridge National Lab, Oak Ridge, TN, ELBIO DAGOTTO, Oak Ridge National Lab, Oak Ridge, TN and University of Tennessee, Knoxville, TN — The one-orbital model for manganites with cooperative phonons has been investigated via large-scale Monte Carlo (MC) simulations. Focusing on electronic density $n = 0.75$, a regime of competition between ferromagnetic (FM) metallic and charge-ordered (CO) insulating states was identified. In the vicinity of the associated bicritical point, colossal magnetoresistance (CMR) effects were observed. These effects appear even in the clean limit, but only by fine tuning parameters, while adding quenched disorder makes the CMR effects robust. The CMR magnitude is much larger than recently reported when randomly distributed polarons form the competing insulator. The crucial role of the superexchange coupling $J_{\pi\pi}$ is discussed. The appearance of CMR effects is shown to be associated with the development of correlations among polarons above the spin ordering temperatures, in agreement with early neutron scattering investigations. These polarons tend to form small regions resembling the charge and spin arrangement of the low-temperature CO insulating state.

Fe-doping-induced charge-orbital ordering in manganese oxides, HIDEAKI SAKAI, KIMINORI ITO, YOSHINORI TOKURA1, Department of Applied Physics, University of Tokyo — We investigated Fe-doping effects on a ferromagnetic metallic crystal, $(La_{1-x}Pr_{0.3})_{0.5}Ca_{0.5}MnO_3$, which locates near the phase boundary to the charge-orbital ordered insulator. It was found that the competing charge-orbital ordering correlation is induced by substituting a small amount of Fe atoms for Mn ones. Such a tendency nicely contrasts with the impurity-induced ferromagnetic metallic phase appearing in the charge-orbital ordered manganites, for example, Cr-doped Nd$_{0.5}$Ca$_{0.5}$MnO$_3$ as intensively investigated for past years. Furthermore, we observed glassy magnetotransport properties as well as diffuse insulator-metal transition, such as magnetic-field annealing effects and long-time relaxation, like a "relaxor ferromagnet".

Fe-doping-induced charge-orbital ordering in manganese oxides, HIDEAKI SAKAI, KIMINORI ITO, YOSHINORI TOKURA1, Department of Applied Physics, University of Tokyo — We investigated Fe-doping effects on a ferromagnetic metallic crystal, $(La_{1-x}Pr_{0.3})_{0.5}Ca_{0.5}MnO_3$, which locates near the phase boundary to the charge-orbital ordered insulator. It was found that the competing charge-orbital ordering correlation is induced by substituting a small amount of Fe atoms for Mn ones. Such a tendency nicely contrasts with the impurity-induced ferromagnetic metallic phase appearing in the charge-orbital ordered manganites, for example, Cr-doped Nd$_{0.5}$Ca$_{0.5}$MnO$_3$ as intensively investigated for past years. Furthermore, we observed glassy magnetotransport properties as well as diffuse insulator-metal transition, such as magnetic-field annealing effects and long-time relaxation, like a "relaxor ferromagnet".

Dirty Peierls transition to stripe phase in manganites, SUSAN COX, National High Magnetic Field Laboratory, Los Alamos National Laboratory, JASON LASHLEY, EDWARD ROSTEN, Los Alamos National Laboratory, ANTHONY WILLIAMS, CSEC, University of Edinburgh, JOHN SINGLETON, National High Magnetic Field Laboratory, Los Alamos National Laboratory, PETER LITTLEWOOD, Cavendish Laboratory, University of Cambridge — The nature of the phase transitions in La$_{0.65}$Ca$_{0.5}$MnO$_3$ and Pr$_{0.45}$Ca$_{0.5}$MnO$_3$ has been probed using heat capacity and magnetisation measurements. The phase transition associated with the onset of the stripe phase has been identified as a second order transition which can be very well fitted by the model of a Peierls transition in a disordered system (a `dirty' Peierls transition). We demonstrate that this model can also be applied to other systems (such as alpha-Uranium) in which Peiers transitions occur.

Weak charge disproportion and leading mechanisms in half-doped manganites, DMITRI VOLJA, WEI GUO YIN, Brookhaven National Laboratory — The puzzling very weak charge disproportion in half-doped manganate such as La$_{1/2}$Ca$_{1/2}$MnO$_3$ is reconciled with the well-accepted Mn$^{3+}$/Mn$^{4+}$ picture of charge and orbital orders via our novel first-principles Wannier function analysis. The strong electron itinerancy is found to delocalize the Mn$^{4+}$ Wannier states significantly, producing remarkable charge leaking into the "Mn$^{4+}$" sites. Thus, it is necessary to distinguish for this charge-transfer system actual charge from the occupation number. Finally, a realistic low-energy effective Hamiltonian is derived, revealing the interesting role of electron-electron interactions in the charge and orbital channels, which can be applied to other doping regions including the CMR phase.

No.
1:03PM Y13.00008 Competing Ferromagnetic and Charge-Ordered States in Realistic Models for Manganites: the Origin of the CMR Effect, CENGIZ SEN, National High Magnetic Field Lab and Florida State University, Tallahassee, FL, GONZALO ALVAREZ, Oak Ridge National Lab, Oak Ridge, TN, ELBIO DAGOTTO, Oak Ridge National Lab, Oak Ridge, TN and University of Tennessee, Knoxville, TN — The one-orbital model for manganites with cooperative phonons has been investigated via large-scale Monte Carlo (MC) simulations. Focusing on electronic density $n = 0.75$, a regime of competition between ferromagnetic (FM) metallic and charge-ordered (CO) insulating states was identified. In the vicinity of the associated bicritical point, colossal magnetoresistance (CMR) effects were observed. These effects appear even in the clean limit, but only by fine tuning parameters, while adding quenched disorder makes the CMR effects robust. The CMR magnitude is much larger than recently reported when randomly distributed polarons form the competing insulator. The crucial role of the superexchange coupling $J_{\pi\pi}$ is discussed. The appearance of CMR effects is shown to be associated with the development of correlations among polarons above the spin ordering temperatures, in agreement with early neutron scattering investigations. These polarons tend to form small regions resembling the charge and spin arrangement of the low-temperature CO insulating state.

1:15PM Y13.00009 Fe-doping-induced charge-orbital ordering in manganese oxides, HIDEAKI SAKAI, KIMINORI ITO, YOSHINORI TOKURA1, Department of Applied Physics, University of Tokyo — We investigated Fe-doping effects on a ferromagnetic metallic crystal, $(La_{1-x}Pr_{0.3})_{0.5}Ca_{0.5}MnO_3$, which locates near the phase boundary to the charge-orbital ordered insulator. It was found that the competing charge-orbital ordering correlation is induced by substituting a small amount of Fe atoms for Mn ones. Such a tendency nicely contrasts with the impurity-induced ferromagnetic metallic phase appearing in the charge-orbital ordered manganites, for example, Cr-doped Nd$_{0.5}$Ca$_{0.5}$MnO$_3$ as intensively investigated for past years. Furthermore, we observed glassy magnetotransport properties as well as diffuse insulator-metal transition, such as magnetic-field annealing effects and long-time relaxation, like a "relaxor ferromagnet".

1:27PM Y13.00010 Dirty Peierls transition to stripe phase in manganites, SUSAN COX, National High Magnetic Field Laboratory, Los Alamos National Laboratory, JASON LASHLEY, EDWARD ROSTEN, Los Alamos National Laboratory, ANTHONY WILLIAMS, CSEC, University of Edinburgh, JOHN SINGLETON, National High Magnetic Field Laboratory, Los Alamos National Laboratory, PETER LITTLEWOOD, Cavendish Laboratory, University of Cambridge — The nature of the phase transitions in La$_{0.65}$Ca$_{0.5}$MnO$_3$ and Pr$_{0.45}$Ca$_{0.5}$MnO$_3$ has been probed using heat capacity and magnetisation measurements. The phase transition associated with the onset of the stripe phase has been identified as a second order transition which can be very well fitted by the model of a Peierls transition in a disordered system (a 'dirty' Peierls transition). We demonstrate that this model can also be applied to other systems (such as alpha-Uranium) in which Peiers transitions occur.

1:39PM Y13.00011 Weak charge disproportion and leading mechanisms in half-doped manganites, DMITRI VOLJA, WEI GUO YIN, Brookhaven National Laboratory — The puzzling very weak charge disproportion in half-doped manganate such as La$_{1/2}$Ca$_{1/2}$MnO$_3$ is reconciled with the well-accepted Mn$^{3+}$/Mn$^{4+}$ picture of charge and orbital orders via our novel first-principles Wannier function analysis. The strong electron itinerancy is found to delocalize the Mn$^{4+}$ Wannier states significantly, producing remarkable charge leaking into the "Mn$^{4+}$" sites. Thus, it is necessary to distinguish for this charge-transfer system actual charge from the occupation number. Finally, a realistic low-energy effective Hamiltonian is derived, revealing the interesting role of electron-electron interactions in the charge and orbital channels, which can be applied to other doping regions including the CMR phase.

1:51PM Y13.00012 Charge separation and giant dielectric response in LSMO, ZSOLT MARTON, Department of Materials Science and Engineering, University of Pennsylvania, RINAT F. MAMIN, Zavoisky Physical-Technical Institute of RAS, Kazan,Russia, TAKESHI EGAMI, Department of Physics and Astronomy, University of Tennessee/Oak Ridge National Laboratory, Oak Ridge — Numerous researches are being applied to other systems (such as alpha-Uranium) in which Peierls transitions occur.

2:03PM Y13.00013 Experimental and theoretical determination of the anisotropic anomalous scattering tensor at the Mn K edge in LaMnO$_3$, JOAQUIN GARCIA, GLORIA SUBIAS, M.C. SANCHEZ, ICMA, CSIC-Universidad de Zaragoza, Spain, J. HERRERO-MARTIN, CMA,CSIC-Universidadaz, Spain de Zarago, KEISUKE HATADA, C.R. NATOLI, S. DI MATTEO, LNF, INFN, Frascati Italy, C. MAZZOLI, ESRF, Grenoble, France, J. BLASCO, ICMA, CSIC-Universidad de Zaragoza, Spain — A resonant x-ray scattering (RXS) study of (h 0 0), (0 k 0) and (0 0 l) forbidden reflections (h, k, l odd) at the Mn K-edge of LaMnO$_3$ was performed between 10 and 300 K. We observed strong resonant peaks at the three reflections. The azimuth angle dependence of all these reflections showed a characteristic sine evolution of $\pi$-period. The energy dependence of the intensity for (h 0 0) and (0 k 0) reflections was identical while different structures were observed for (0 0 l) reflections. We did not observe any change either on the resonance intensity or on the line shape when crossing the Néel temperature $T_N \sim 140$ K. The energy, azimuth angle and polarization dependences of the three reflections are originated by off-diagonal terms of the scattering tensor. The theoretical analysis show that the principal axes of the anomalous scattering tensor depends on the photon energy. Moreover, resonant scattering in LaMnO$_3$ is not a probe of d-orbital ordering.
11:15AM Y14.0001 InAs quantum well Hall devices for room-temperature detection of magnetic biomolecular labels1, GORAN MIHAJLOVIC2, MARTECH and Department of Physics, Florida State University — The integration of micro- and nanoscale magnets with molecular biology promises novel applications in fundamental studies of molecular interactions as well as in bioanalysis and biomedical functions. The implementation of this concept requires detection of biomolecular labels in the form of superparamagnetic micro/nano beads, ideally with single bead sensitivity. In this talk we will present our development of miniaturized Hall sensors for detection of such beads. The devices, with Hall cross widths of ∼1 µm and ∼250 nm, were fabricated from InAs/AlSb quantum well semiconductor heterostructures. Their room-temperature characteristics were examined by Hall effect and electronic noise measurements. In the low frequency range, from 20 Hz to 1.6 kHz, devices have the noise-equivalent magnetic moment sensitivities of order $10^{-7} \mu_B/\sqrt{Hz}$ and $10^{-6} \mu_B/\sqrt{Hz}$ respectively. The sensitivity of the latter reaches the $10^{-5} \mu_B/\sqrt{Hz}$ range above ∼1 kHz. By using a phase-sensitive measurement technique and micron-sized Hall crosses we achieved detection of a single 1.2 µm diameter bead with a signal to noise ratio (S/N) of ∼3.3 dB, as well as detection of six 250 nm beads with S/N of ∼2.3 dB per bead. Our results from the micro-Hall susceptibility measurement on a single microbead can be explained quantitatively as due to the magnetic response of an ensemble of non-interacting magnetic nanoparticles with broad distribution of magnetic moments. The work demonstrates the efficacy of InAs quantum well Hall devices for applications in high sensitivity magnetic biomolecular detection.

1Work done in collaboration with P. Xiong, S. von Molnar, M. Field, G.J. Sullivan, K. Ohtani, and H. Ohno, and supported by NSF NIRT Grant ECS-0210332.

2Present address: Materials Science Division, Argonne National Laboratory

11:51AM Y14.0002 Superparamagnetic bead assembly via biomolecular recognition and detection using micro Hall sensor1, PRADEEP MANANDHAR, GORAN MIHAJLOVIC, STEPHEN VON MOLNAR, PENG XIONG, MARTECH & Department of Physics, Florida State University, KEITA OHTANI, HIDEO OHNO, Laboratory for Nanoelectronics and Spintronics, Tohoku University, MARK FIELD, GERARD J. SULLIVAN, Teledyne Scientific Company — Specific binding of biological molecules onto a selectively functionalized area is a necessary key step in biological sensing with a solid state device. Here we present our results on the directed self-assembly of streptavidin coated superparamagnetic micro and submicron sized beads onto selectively biotinylated solid-state surfaces with organic molecular templates. Large-scale high-yield assembly of 130nm streptavidin-coated beads onto biotinylated micro-patterns with little nonspecific binding is realized using molecular template generation by micro-contact printing. Specific binding of similar beads onto a semiconductor micro-Hall cross can be realized using high-spatial registry functionalization with dip-pen nanolithography, and the binding can be detected using phase sensitive Hall magnetometry with InAs quantum well micro-Hall sensors.

1Work supported by NSF NIRT grant ECS-0210332.

G. Mihajloviæ et al., APL 87, 112502 (2005).

12:03PM Y14.0003 In-vitro heating with Polyethylene Glycol Coated Magnetic Nanoparticles, Srinivasan Balakrishnan, M.J. Bonder, D. Gallo, G. C. Hadjipanayis, Department of Physics and Astronomy, University of Delaware — Magnetic nanoparticle systems synthesized with a biocompatible polymer coating are under investigation for future detection and treatment of cancer. In this study we investigate the heating characteristics of Fe based nanoparticles coated with polyethylene glycol. Structural characterization indicates a variation in the composition with polymer concentration. The x-ray analyses show that samples become increasingly amorphous as evidenced by the broad amorphous-like peak superimposed on the alpha iron (110) peak. The magnetization curves indicate that all samples are soft ferromagnets with the coercivity dependent on mean particle size. When the nanoparticle suspension is subjected to a 4Oe, 500 kHz AC magnetic field there is a steep rise in temperature reaching an equilibrium temperature for all cases. Correlating the equilibrium temperature with the static magnetic properties shows that the temperature is linearly dependent on the saturation magnetization and inversely proportional to the coercivity of the particle. Work supported by NSF DMR-0302544.

12:15PM Y14.0004 Ferromagnetic Gd$_{100-x}$Fe$_x$ (x = 4 - 40) Nanostructures, D. Schmitter, J. Goertzen, G. SHELBURNE, University of Nebraska - Lincoln, T. M. Pekarek, University of North Florida, J. E. SHIELD, University of Nebraska - Lincoln, P. M. SHAND, University of Northern Iowa, D. HASKEL, Argonne National Laboratory, D. L. Lesieiev-Pelecky, University of Nebraska - Lincoln — Iron in concentrations as small as 4 at. % (where the distance between Fe atoms is more than three lattice spacings) produces ferromagnetic behavior at temperatures up to 50 K above the Gd Curie temperature $T_C$ in Gd$_{100-x}$Fe$_x$ nanostructures. X-ray diffraction and XAFS show that Gd$_{100-x}$Fe$_x$ nanostructures made by inert-gas-condensation and melt-spinning have nanoscale hcp Gd grains with Fe-Gd grain boundaries. Magnetization and XMCD measurements indicate that, above the bulk Gd $T_C$, Fe atoms polarize Gd atoms and produce ferromagnetic behavior with coercivities on the order of 50-100 Oe. The coercivity decreases as the temperature decreases toward the Gd $T_C$, which we attribute to random anisotropy averaging produced by ordering of the hcp-Gd grains.

12:27PM Y14.0005 Geometrically frustrated honeycomb and ladder lattices of nanoscale ferromagnetic islands, JIE LI, XIANGLIN KE, RUIFANG WANG, WILLIAM MCCONVILLE, CRISTIANO NISOLI, PAUL LAMMERT, VINCENT CRESPI, PETER SCHIFFER, The Penn State University — We have studied arrays of interacting single-domain ferromagnetic islands which are arranged on lattices such that the interactions between the islands are frustrated by the geometry of the arrays. While previous studies in our group [1] have focused on a frustrated square lattice, we now report results on lattices with the honeycomb geometry and with a topologically equivalent ladder geometry in which the islands meet in vertices of three islands. Each permalloy island measures approximately 80nm by 220nm with a thickness 25nm, and is evenly spaced with lattice spacing ranging from 225nm to 425nm for honeycomb lattice and from 320nm to 880nm for ladder lattice. Magnetic force microscopy measurements of the arrays after demagnetization show that the interactions between the islands are frustrated and that the correlations between islands decrease with increasing spacing of the islands. A detailed analysis of the correlations between the islands will be presented. This research has been supported by the Army Research Office. [1] R. F. Wang, C. Nisoli, R. S. Freitas, J. Li, W. McConville, B. J. Cooley, M. S. Lund, N. Samarth, C. Leighton, V. H. Crespi, and P. Schiffer, Nature 439, 303 (2006).

12:39PM Y14.0006 Field annealing study of a frustrated interacting nanomagnet array1, X. KE, J. LI, W. MCCONVILLE, R. WANG, C. NISOLI, P. LAMMERT, V. CRESPI, P. SCHIFFER, Dept. of Physics and Materials Research Institute, Pennsylvania State University, University Park, PA, 16802 — Lithographically patterned ferromagnetic nano-islands provide an ideal model to explore the physics of frustrated ‘spin ice’ materials due to the competition of dipole interaction between elements [1]. Since the energy scales are large compared to thermal energies, field annealing is crucial to obtaining a low-energy demagnetized state among the interacting islands. We have studied various field annealing protocols to demagnetize the array by rotating the sample in a time-varying magnetic field. We find that reversing the field direction while stepping down the field magnitude is needed for successfully demagnetize the array. The annealing can also be tuned by varying the field step size, especially for field magnitudes near the coercive field of the array. The competition of dipole interaction with external field and dipole field of neighboring elements will be discussed.

1We acknowledge financial support from Army Research Office and the National Science Foundation MRSEC program.
12:51PM Y14.00007 Magnetic domain wall phases in perpendicularly magnetized ultrathin films. . . NIDAL ABU-LIBDEH, DAVID VENUS, Department of Physics and Astronomy, McMaster University — At low temperature, the ground state of a perpendicularly magnetized ultrathin film is the striped state with equilibrium magnetization \( m \) of domain walls that runs transverse to the applied magnetic field with an equilibrium magnetic susceptibility \( \chi \) of \( \sim 1/m \). The change in domain density with temperature involves the creation/annihilation of domain walls. We propose a simple relaxation model in which the domain wall creation/annihilation is an activated process. The model predicts a non-equilibrium domain density and thus an effective susceptibility that depends on the time scale of the measurements. We have measured the ac-magnetic susceptibility of perpendicularly magnetized ultrathin Fe films on a 2 ML Ni/W(110) substrate, as a function of temperature while changing the temperature at different heating rate \( R \) between 0.03K/s and 1K/s. In the low temperature range, the model calculations provide a consistent explanation of the measured susceptibility. In the high temperature range, the susceptibility measured with low heating rates (0.03K/s - 0.1K/s) deviates from the calculation due to an increase of the high temperature half-width of the susceptibility. This has been tentatively interpreted as a phase change from the stripe domain phase to the tetragonal phase in which the domains have no preferred direction.

1:03PM Y14.00008 Magnetization Reversal in Europium Sulfide Nanocrystals. JAMES DICKERSON, MARCELKA REDIGOLO, Dept. of Physics and Astronomy, Baylor University, DMITRY KOKTYSYH, Dept. of Chemistry, Vanderbilt University, SANDRA ROSENTHAL, Dept. of Chemistry and Dept. of Physics and Astronomy, Vanderbilt University, ZHENGI GAI, Center for Nanophase Materials Science & Materials Science and Technology Division., Oak Ridge National Laboratory, LAN GAO, Center for Nanophase Materials Science Division, Oak Ridge National Laboratory, JIAN SHEN, Center for Nanophase Materials Science & Materials Science and Technology Division., Oak Ridge National Laboratory — We report the observation of the reversal in the magnetization hysteresis curve of europium sulfide nanocrystals. This phenomenon was investigated through the temperature-dependent magnetization of two classes of nanomaterials, nanocrystalline (2.0 nm \( \leq \) d_{NCs} \leq 100 nm), and quantum-confined (d_{NCs} \leq 2.0 nm), where d_{NCs} is the diameter of the nanomaterial. The effect of the size of the nanomaterial on the magnetization is attributed to the competition between the magnetic properties of strained surface atoms and unstrained core atoms. Superconducting quantum interference device (SQUID) probing the magnetic response. Electron microscopy and X-ray diffraction spectroscopy revealed the crystallinity and monodispersivity of the nanomaterials.

1:15PM Y14.00009 Magnetism and C NMR relaxation of nanodiamond powder. E.M. LEVIN, Ames Laboratory (AL) and Dept. of Physics and Astr., Iowa State University (ISU), S.L. BUD’KO, AL and Dept. of Physics and Astr., ISU, X.W. FANG, Dept. of Chemistry, ISU, W.E. STRASZHEIM, Materials Analysis and Research Laboratory, ISU, R.W. MCCALLUM, AL and Dept. of Materials Science and Engineering, ISU, K. SCHMIDT-ROHR, Dept. of Chemistry and AL, ISU — The magnetization, C NMR relaxation, and composition of commercial nanodiamonds with an average grain diameter of 4 nm have been studied. The magnetization contains several contributions due to (1) the diamagnetic effect of core and valence electrons of carbon, (2) ferromagnetic-like and (3) superparamagnetic contributions from Fe-bearing particles detected in nanodiamonds, and (4) a paramagnetic contribution from unpaired electrons. The spin concentration obtained from the paramagnetic susceptibility is \( 2.2 \times 10^{20} \) spins/g. At 300 K, nanodiamond powder shows ferromagnetic magnetization of 0.01 emu/g. C NMR spectra and relaxation times should be unaffected by the ferromagnetic particles with so small magnetization. Thus, a reduction of C NMR T2 relaxation times by orders of magnitude compared to microdiamond can be explained by unpaired electrons in the nanodiamond grains. The origins of unpaired electrons and ferromagnetism in nanodiamond powder and other carbon-based materials are discussed in view of our results.

1:27PM Y14.00010 Magnetic Endohedral Metallofullerenes with Floppy Interiors. MEICHUN QIAN, SHIV KHANNA, Virginia Commonwealth University, MARK KNICKELBEIN, Argonne National Laboratory — Investigations on the electronic structure and magnetic properties of a free Gd\textsubscript{13}N and Gd\textsubscript{13}N\textsubscript{100}C\textsubscript{80} have been carried out using x-ray microsopy to examine the stability and the electronic and magnetic properties of the endohedral species. Using a synergistic approach combining Stern-Gerlach experiments in beams and first principles electronic structure studies, it is demonstrated that an isolated Gd\textsubscript{13}N has a ground state spin moment of 23 \( \mu \text{B} \) followed by a non-collinear state of 17.2 \( \mu \text{B} \) only 88 meV above the ground state. The large moment is largely due to localized f-electrons. As a Gd\textsubscript{13}N is embedded inside a C\textsubscript{60} cage, the localized f-electrons maintain the magnetic character while the hybridization between the d-s states of isolated Gd\textsubscript{13}N and p-states of C\textsubscript{60} leads to a strongly bound motif with an interaction energy of 13.63 eV and a large HOMO-LUMO gap of 1.48 eV. Gd\textsubscript{13}N\textsubscript{100}C\textsubscript{80} is further shown to possess two isomers corresponding to the location of the N atom on either side of the Gd\textsubscript{13} triangle with an appreciable electric dipole moment and a low barrier of 91 meV for transition between them offering potential for a fluctuating dipole.

1:39PM Y14.00011 Can Carbon Be Ferromagnetic - X Rays Can Give The Answer. HENDRICK OHLDAG, Stanford Synchrotron Radiation Laboratory, TOLEK TYLISZCZAK, Lawrence Berkeley National Laboratory, ROLAND HOHNE, DANIEL SPE-MANN, PABLO ESQUINAZ, MAGDA UNGURENEAU, TILMAN BUTZ, University of Leipzig — Magnetic properties of Ni nanoparticles used for vertically-aligned carbon nanofiber (VACNF) synthesis are investigated. Ni thin films are deposited on Si wafers by sputter-depositing to thicknesses of 2–10 nm. The VACNFs are then grown in a Plasma-Enhanced Chemical Vapor Deposition (PECVD) chamber with NH\textsubscript{3} and C\textsubscript{2}H\textsubscript{2} at relative flow rates of 80/40 sccm, respectively, a pressure of 3 Torr, and a temperature of 700°C. The catalyst particles, after nanofiber growth, are 10–150 nm in diameter. Magnetic properties, after investigation by SQUID magnetometry in applied magnetic fields of \( |H| < 10 \text{ Koe} \) and temperatures \( T = 5–300 \text{ K} \). The catalyst particles are ferromagnetic with low coercivity and remanence. The ferromagnetic properties are thermally stable up to room temperature in all but the smallest particle sizes. Saturation magnetization is much less than would be expected from the deposited quantity of Ni metal.

1:51PM Y14.00012 Magnetic Properties of Ni Nanoparticles Used for Carbon Nanofiber Synthesis. K. D. SORGE, O. MALKINA, C. FINKEL, Florida Atlantic University, J. D. FOWKLES, P. D. RACK, University of Tennessee, K. L. KLEIN, A. V. MELECHKO, M. L. SIMPSON, Oak Ridge National Laboratory — Magnetic properties of Ni catalyst particles used for vertically-aligned carbon nanofiber (VACNF) synthesis are investigated. Ni thin films are deposited on Si wafers by sputter-depositing to thicknesses of 2–10 nm. The VACNFs are then grown in a Plasma-Enhanced Chemical Vapor Deposition (PECVD) chamber with NH\textsubscript{3} and C\textsubscript{2}H\textsubscript{2} at relative flow rates of 80/40 sccm, respectively, a pressure of 3 Torr, and a temperature of 700°C. The catalyst particles, after nanofiber growth, are 10–150 nm in diameter. Magnetic properties, after investigation by SQUID magnetometry in applied magnetic fields of \( |H| < 10 \text{ Koe} \) and temperatures \( T = 5–300 \text{ K} \). The catalyst particles are ferromagnetic with low coercivity and remanence. The ferromagnetic properties are thermally stable up to room temperature in all but the smallest particle sizes. Saturation magnetization is much less than would be expected from the deposited quantity of Ni metal.

This work was supported by the Material Sciences and Engineering Division Program of the U.S. DOE Office of Science. A portion of this research was conducted at the CNMS.
Moving magnetic nanoparticles through soft-hard magnetic composite system

HEMACHANDER SUBRAMANIAN, JONG HAN, State University of New York at Buffalo — An important requirement during the design of a nano-electromechanical system is the ability to move a nanoparticle from one point to another in a predictable way. Through simulations, we demonstrate that soft-hard magnetic structures can help us move nanoparticles predictably. We simulated a 2-D system, in which the exchange-coupled soft-magnetic magnetization is frustrated with the boundary condition set by a hard magnetic array and rotating external field. We consider a geometry with three-fold degenerate magnetic local minima and show that the hysteretic transitions are manipulated by an external field. Due to the reduced interfacial energy from weak demagnetization energy in the composite magnets and magnetic hysteresis, the energy landscape can be manipulated in a well-defined and predictable manner. We apply this idea to control the movement of a magnetic particle placed on a non-magnetic layer on top of the structure. We are interested in extending this simple, preliminary study to include complex geometries. We expect that complex geometrical constraints would lead to interesting orbits of nanoparticles in these systems.

1Supported by NSF DMR-0426826