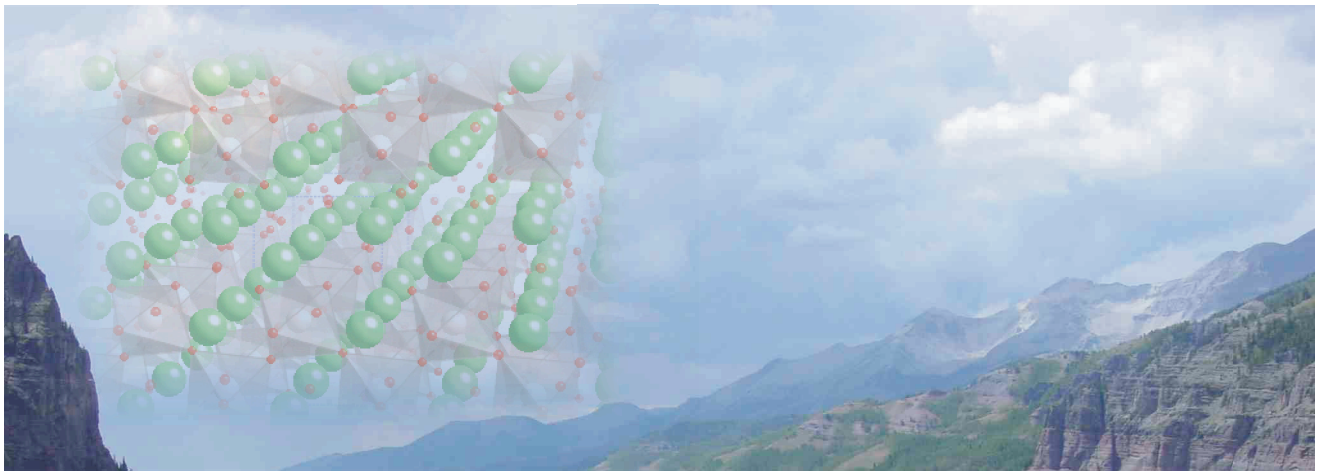

Competing Interactions and Colossal Responses in Transition Metal Compounds

July 16-22 2006
Telluride, CO

Workshop Program

Sunday, July 16, 2006

6:30pm Welcome Reception
Blue Point Grill & Noir Bar ~ 123 S. Oak St, Telluride

Monday, July 17, 2006

8:30am Welcome and Introduction
Ray Osborn and Simon Billinge

Chair: Dan Dessau

8:45am Atomic-scale crystalline and electronic structures of perovskite and bilayer manganites
Christoph Renner ~ London Centre for Nanotechnology

9:15am Atomic scale characterization of manganites and cuprates by electron microscopy: where are the limits?
Maria Varela ~ Oak Ridge National Laboratory

9:45am Unexpected Complexity in the Phase Diagram of Bilayer Manganites
Ken Gray ~ Argonne National Laboratory

10:15am Coffee Break

Chair: Chris Leighton

10:45am Correlations between local structure and magnetization - constraints on domain structure
Frank Bridges ~ University of California, Santa Cruz

11:15am Influence of crystal superstructure and atomic steps in the magnetism of manganite films
Yeong-Ah Soh ~ Dartmouth College

11:45pm Unbiased numerical studies of realistic Hamiltonians for diluted magnetic semiconductors
Adriana Moreo ~ University of Tennessee

12:15pm Magnetic field induced magnetic phase separation in random antiferromagnets
Phil Duxbury ~ Michigan State University

Tuesday, July 18, 2006

Chair: Adriana Moreo

8:45am ARPES investigations of the layered manganites
Dan Dessau ~ University of Colorado

9:15am Nodal quasiparticle in pseudogapped colossal magnetoresistive manganites
Norman Mannella ~ Stanford University

9:45am The Role of Nesting in Bilayer Manganites
Michael Norman ~ Argonne National Laboratory

10:15am Coffee Break

Chair: Ken Gray

10:45am About the Origin of Polaron Correlations in Bilayer Manganites
Stephan Rosenkranz ~ Argonne National Laboratory

11:15am Short-range antiferromagnetic fluctuations and polaron correlations in the layered CMR manganites
Toby Perring ~ ISIS Pulsed Neutron Facility

11:45am Monte Carlo Study of the Resistivity in Spin-fermion Models for Colossal Magnetoresistive Manganites
Gonzalo Alvarez ~ Oak Ridge National Laboratory

12:15pm Connecting Mn-O Hybridization to the Electronic Properties of Manganites
John Freeland ~ Argonne National Laboratory

6:30pm **Evening Discussion**
Disorder: Measurements, Models and Reality
Chair: Simon Billinge

Wednesday, July 19, 2006

Chair: Jaime Fernandez-Baca

8:45am Charge Ordering and Ferroelectricity in Oxides
Daniel Khomskii ~ University of Cologne, Germany

9:15pm Competition of local and long-range polar order in relaxor ferroelectrics
Guangyong Xu ~ Brookhaven National Laboratory

9:45am Recent Results on CMR and Multiferroic Manganese Oxides
Jeff Lynn ~ NIST Center for Neutron Research

10:15am Coffee Break

Chair: John Mitchell

10:45am The great impact of substitution upon the electrical and magnetic states of metal-transition perovskite oxides
Antoine Maignan ~ CNRS/ENSICAEN, France

11:15am Spontaneous rotation of orbital stripes and ferroelectric state in bilayer manganites
Yusuke Tokunaga ~ ERATO-SSS, JST, Japan

11:45am Multiferroic behavior in RMn_2O_5 materials (R=Y,Tb)
Laurent Chapon ~ ISIS Pulsed Neutron Facility

12:15pm A simple model for magneto-electric effect in non-collinear magnets
Bhanu Mahanti ~ Michigan State University

6:30pm **Evening Discussion**
Commonalities in the Electronic Structure of Transition Metal Oxides
Chair: Michael Norman

Thursday, July 20, 2006

Chair: Stephan Rosenkranz

9:00am Structural and Magnetic Properties of the Extended Kagomé Antiferromagnet $RBaCo_4O_7$ (R=Y,Yb,Tm,Lu)
John Mitchell ~ Argonne National Laboratory

9:30am Intrinsic nanometer-scale electronic phase separation and simple percolation in doped cobaltites
Chris Leighton ~ University of Minnesota

10:00am The true magnetic nature of CMR Cobaltites
Despina Louca ~ University of Virginia

10:30am Coffee Break

Chair: Jeff Lynn

11:00am Dance of Electrons on a Triangular Lattice (Na_xCoO_2)
Zahid Hasan ~ Princeton University

11:30am Orbital Ordering in Layered Ruthenates
Christie Nelson ~ Brookhaven National Laboratory

12:00pm Temperature Dependent Bilayer Ferromagnetism in $Sr_3Ru_2O_7$
Matthew Stone ~ Oak Ridge National Laboratory

6:00pm **Workshop BBQ Picnic**

Friday, July 21, 2006

Chair: Despina Louca

9:00am Frustrated spinels under extreme conditions
Seunghun Lee ~ University of Virginia

9:30am Spontenaous spin-lattice coupling in the geometrically frustrated triangular lattice antiferromagnet $CuFeO_2$
Jaime Fernandez-Baca ~ Oak Ridge National Laboratory

10:00am *Gabriel Aeppli* ~ London Centre for Nanotechnology

10:30am Coffee Break

Chair: Ray Osborn

11:00am "Surprise Talk"
Simon Billinge ~ Michigan State University

11:30am Workshop Summaries and Discussion

12:30pm Conclusion of Workshop

Workshop Participants

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Atomic-scale crystalline and electronic structures of perovskite and bilayer manganites*

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A detailed characterization of the electronic and crystalline structures of manganites is of primary interest in the quest for a microscopic model describing the extraordinary transport properties of these complex ceramics. The most remarkable one, the negative colossal magnetoresistance, develops in the vicinity of a metal insulator transition where strong phase competition is expected to take place. We shall review scanning tunneling microscopy and spectroscopy experiments we performed on a pseudocubic perovskite† and a bilayer‡ manganite. In both systems, we find different phases coexisting in single crystals and thin films, from charge-ordered checkerboard to stripes and hexagonal impurity phases. But to date, we have not found any experimental evidence of electronic phase separation where electronic charge is segregating on nanometer lengths scales in an otherwise chemically homogeneous lattice. We also present a possible real space glimpse of a small polaron in a bilayer manganite‡, that very elusive object whose peculiar dynamics might be responsible for its remarkable transport properties.

*Collaboration with H.M. Rønnow, G. Aeppli, and B. Bryant.
†Ch.Renner, G.Aeppli, B-G.Kim, Yeong-Ah Soh, and S.-W.Cheong, Nature **416**, 518 (2002).
‡H.M.Rønnow, Ch.Renner, G.Aeppli, T.Kimura, and Y.Tokura, Nature **440**, 1025 (2006).

Atomic scale characterization of manganites and cuprates by electron microscopy: where are the limits?

M. Varela[1], J. Tao[1], A.R. Lupini[1], S.J. Pennycook[1], W. Luo[2], S.T. Pantelides[2], V. Peña[3], J. García-Barriocanal[3], Z. Sefrioui[3], C. León[3], J. Santamaría[3]
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Epitaxial complex oxide ultrathin films and heterostructures constitute ideal systems to study the nature and effects of inhomogeneity and phase separation. Perovskite oxides can be chosen with similar lattice parameters and good chemical compatibility which allows high quality, epitaxially coherent growth. But the reduced dimensionality and the presence of interfaces and epitaxial strain may also cause new phenomena to arise. It is desirable to have a comprehensive study of the relations between structural, chemical and electronic properties at the atomic scale. For this aim, the combination of aberration-corrected scanning transmission electron microscopy, energy-loss spectroscopy and first-principles theory provides a powerful tool to analyze these relationships with atomic resolution. This work reviews recent results on oxides and presents several studies on manganite and cuprate thin films and interfaces. Examples include charge ordering, hole localization and phase separation.
This research was sponsored by the LDRD Program of ORNL, managed by UT-Batelle, LLC, for the U.S. DOE under Contract No. DE-AC05-00OR22725 and by the Spanish CICyT, Mat2005-06024-C02.

Unexpected Complexity in the Phase Diagram of Bilayer Manganites

K.E. Gray, Qing'An Li, H, Zheng, H. Claus, S. Rosenkranz, S. Nyborg Ancona, R. Osborn, J.F. Mitchell
Materials Science Division, Argonne National Laboratory, Argonne, IL 60439

Important modifications to the phase diagram of the layered manganites have been discovered through combined conductivity, magnetization and neutron and x-ray diffraction. Contrary to conventional wisdom, purified LaSr2Mn2O7 crystals (x=0.5) exhibit CE-type orbital and charge order as the low-temperature ground state. For small deviations from x=0.5, the high temperature CE phase is replaced at low temperatures by an A-type antiferromagnet 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 re-entrance with coexistence. For x=0.6, conductivity, magnetization and scattering data show a first-order transition from a bistripe orbital/charge-ordered insulator to a metal as the temperature falls below 160 K. This result supports a contention that strongly coupled magnetic/conductive transitions are universally of 1st order.

Correlations between local structure and magnetization - constraints on domain structure

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[2] *Physics Dept. Montana State University, Bozeman, MT 59717, USA*
[3] *Argonne National Laboratory, Argonne, Illinois 60439, USA*

For the colossal magnetoresistive manganites we have observed a correlation between the magnetization, $\mathbf{M}$(T), and changes in the local structure $\Delta(\sigma^2)$(T), where σ is the width of the Mn-O pair distribution function. This correlation is the same through the transition (or cross-over), independent of whether we change $\mathbf{M}$ by decreasing the temperature or by increasing an applied magnetic field $\mathbf{B}$. A common feature is that the distortion removed/(Mn-site), as T drops below T_c or $\mathbf{B}$ is increased, is small until $\mathbf{M}/\mathbf{M}_o > 50\%$ ($\mathbf{M}_o$ is the saturation magnetization). Above $\mathbf{M}/\mathbf{M}_o \sim 2$x, (twice the hole conc.), the distortion removed/(Mn-site) increases rapidly with $\mathbf{M}$. Consequently, the quasiparticles that initially aggregate to form magnetic domains have little static distortion that is removed upon magnetization; most of the distortion is found on the sites that become magnetized when $\mathbf{M}$ is high. We refer to the smallest such quasiparticle as a dimeron - a hole (or electron) localized on two Mn sites. This leads to a filamentary nature for any domain formation and suggests that in the magnetization process the order in which sites become magnetized is not random; we suggest this is a result of the quenched-in disorder from the random location of the Ca or Sr dopant atoms. Irrespective of which pairing model is favored, it must include this correlation between changes in the local lattice distortion and the sample magnetization. Some consequences of these paired clusters are discussed.

Influence of crystal superstructure and atomic steps in the magnetism of manganite films

Yeong-Ah Soh
Dartmouth College, Department of Physics and Astronomy, Hanover, NH 03755, USA

$La_{0.7}Sr_{0.3}MnO_3$ films grown on $SrTiO_3$ exhibit magnetic texture within magnetic domains. In this talk, I will show that the magnetic texture is due to the crystal superstructure that self assembles in manganite films in order to accommodate the strain from the lattice mismatch with the substrate. As a comparison, we have performed studies on $La_{0.7}Sr_{0.3}MnO_3$ films grown on $NdGaO_3$, which are nominally strain free. No magnetic texture is observed in these films. In addition, magnetic contrast is observed only near the Curie temperature, where magnetization at the step terraces differs from magnetization at the step edges.

Unbiased numerical studies of realistic Hamiltonians for diluted magnetic semiconductors

Adriana Moreo
Department of Physics and Astronomy,University of Tennessee, Knoxville, TN 37966-1200 and Condensed Matter Sciences Division, Oak Ridge National Laboratory,Oak Ridge, TN 37831-6032

We formulated a real space Hamiltonian to study the effect of dilute magnetic doping of III-V semiconductors. A p-type valence band is considered and nearest neighbor hopping of holes among bonding orbitals in a diamond lattice is allowed. The relevant hopping parameters between orbitals are obtained in terms of the Luttinger parameters. Considering the effects of the spin-orbit interactions the number of degrees of freedom per site is reduced from 6 (3 orbitals and two spin orientations for the p bands) to 4 (the four projections corresponding to j=3/2 which is the quantum number of the heavy and light hole bands). The magnetic interaction between the doped magnetic impurities and the spin of the mobile holes is written in the appropriated base. The numerical values of the hopping parameters and Hund interaction are obtained from the literature for the different compounds and, thus, there are no free parameters. The properties of the materials are calculated using numerical techniques. The newly developed TPEM method allows us to consider lattices with NxNxN cubes with N as big as 6. Since there are 4 ions associated to each site of a cube in an fcc lattice the total number of Ga sites in our simulations is 4xNxNxN. Finite size effects are very small when systems larger than 3x3x3 cubes are considered. For Mn doped GaAs we reproduce the experimentally observed Curie temperatures for all the studied values of effective hole dopings. The accepted value for J=1.2eV corresponds to weak coupling since impurity bands above the top of the valence band are not observed. These bands form for much larger values of J. Results for other magnetically doped III-V compounds will be presented.

Magnetic field induced magnetic phase separation in random antiferromagnets

Phil Duxbury
Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824

We show that a classical model for the bcc diluted antiferromagnet iron-zinc-difluoride exhibits magnetic phase separation as a function of an applied field. In the low field regime a single antiferromagnetic phase exists, while at intermediate fields a percolating cluster of antiferromagnetic order co-exists with a percolating cluster of ferromagnetic order.

ARPES investigations of the layered manganites

Dan Dessau[1], Zhe Sun[1], Fraser Douglas[1], Alexei Fedorov[2], Yi-De Chuang[2], Tsuyoshi Kimura[3], Yoshi Tokura[3], Helen Zheng[4], John Mitchell[4]

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[4] *Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA*

I will discuss the doping and temperature dependence of the measured k-dependent electronic structure of the layered manganites. Important concepts will be the Fermi surface nesting vectors, pseudogaps, electron-phonon coupling, and electronic phase separation.

Nodal quasiparticle in pseudogapped colossal magnetoresistive manganites

N. Mannella
Stanford University and LBNL

In this talk, I will discuss the results of some recent angle-resolved photoemission spectroscopy (ARPES) investigations which allowed elucidating the controversial nature of the ferromagnetic metallic groundstate in the prototypical CMR bilayer compound $La_{1.2}Sr_{1.8}Mn_2O_7$*. The distribution of spectral weight in momentum space exhibits a nodalantinodal dichotomous character. Quasiparticle excitations have been detected for the first time along the nodal direction (i.e. diagonal), and they are found to determine the metallic transport properties of this compound. These nodal quasiparticles coexist with strong anisotropic electron-boson interactions. The weight of the quasiparticle peak diminishes rapidly while crossing over to the antinodal (i.e. parallel to the MnO bonds) parallel sections of the Fermi surface. In particular, the spectra along the antinodal straight sections of the Fermi surface strongly resemble those found in heavily underdoped cuprates high temperature superconductors such as $Ca_{2-x}Na_xCuO_2Cl_2$†. This dichotomy between the electronic excitations along the nodal (diagonal) and antinodal (parallel to the CuO bonds) directions in momentum space was so far considered a characteristic unique feature of the copper oxide high-temperature superconductors (HTSC). These findings therefore cast doubt on the assumption that the pseudogap state and the nodal-antinodal dichotomy in the copper oxides HTSC are hallmarks of the superconductivity state.

*N. Mannella et al., Nature **438**, 474 (2005)
†K. M Shen et al., Science **307**, 901 (2005)

The Role of Nesting in Bilayer Manganites*

M. R. Norman
Materials Science Division
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Recent angle resolved photoemission data have indicated the possibility of Fermi surface nesting that might give rise to the incommensurate charge ordering peaks that have been seen above the Curie temperature by diffuse scattering in the bilayer manganites. To investigate this, we have performed local spin density approximation calculations of the electronic structure for the bilayer manganites, and then calculated the susceptibility by use of a linear tetrahedron scheme. Cusps are observed in the susceptibility at incommensurate wavevectors which do indeed correspond to nesting. We discuss how these cusps vary with momentum as a function of hole doping and the form of the magnetic order (paramagnetic, ferrromagetic, and antiferromagnetic). Implications of our results for ARPES, diffuse scattering, and infrared conductivity studies will be discussed.

*Work supported by the US Dept. of Energy, Office of Science, under Contract W-31-109-ENG-38

Short-range antiferromagnetic fluctuations and polaron correlations in the layered CMR manganites

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Two distinct short-range orderings nanoscale polaron correlations, and antiferromagnetic fluctuations were independently discovered a few years ago in the layered CMR manganites $La_{2-2x}Sr_{1+2x}Mn_2O_7$, x=0.4. Results will be presented of a comprehensive study of both the temperature and magnetic field dependency of the two phenomena for x=0.30 and x=0.35 which also have ferromagnetic intra-layer magnetic ordering. The antiferromagnetic fluctuations seen earlier for x=0.40 are also observed in samples of x=0.30 and x=0.35, and coexist with the ferromagnetic critical scattering. Just as for x=0.4, they appear very rapidly on warming through the three-dimensional ordering temperatures, T_{Crit}, of 90K and 121K respectively, and the intensity tracks that of the resistivity both as a function of magnetic field and temperature for the two compositions. Polaron correlations were measured in the two samples, which occur at wavevectors ($\pm\delta$,0,$\pm$1) δ=0.25, 0.30 for x=0.30, 0.40, and similarly show a magnetic field and temperature dependency of the intensity that tracks the resistivity. The results indicate that both the antiferromagnetic fluctuations and polaron correlations are related phenomena in the layered CMR manganites.

Monte Carlo Study of the Resistivity in Spin-fermion Models for Colossal Magnetoresistive Manganites

Gonzalo Alvarez[1], Elbio Dagotto[2], Cengiz Sen[3]

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[2] *Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 32831 and Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996*
[3] *National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, FL 32310*

This talk presents results of an extensive numerical study on the transport and magnetoresistance of magnetically ordered phases in manganites. These results were obtained with a one-orbital and two-orbital spin fermion model with and without the inclusion of phonons. To treat the fermionic problem we have used exact diagonalization as well as a polynomial expansion method that scales linearly with the lattice size and, therefore, allows us to study large lattices.
In the first part, the discussion will focus on the resistivity maximum with temperature found in our simulations of ferromagnetic manganites and on the effect of an applied magnetic field. In the second part, the effect of quenched disorder on the A-type antiferromagnetic and the CE phases of manganites will be addressed. Monte Carlo simulations give convincing evidence for the occurrence of an insulator to metal transition when disorder is present. Finally, I will discuss the problem of finding a resistivity maximum in cases where the competing states are not both ferromagnetic.

Connecting Mn-O Hybridization to the Electronic Properties of Manganites*

J.W. Freeland[1], K.E. Gray[2], M. van Veenendaal[3], H. Zheng[2], J.F. Mitchell[2]
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Hybridization between oxygen and transition metals plays an important if not crucial role in the behavior of all of the complex oxide systems. The ground state in these systems always contains a fraction of *3d-2p* hybridized states, which play a role in controlling the properties. In the case of cuprates, the formation of coherent *3d-2p* hybridized states (Zhang Rice singlet) are believed to play a crucial part in determining the electronic behavior. For the case of manganites, the case is less clear and has not been studied in depth. One can use bulk sensitive soft x-ray spectroscopy at the oxygen K edge, to probe holes with 3d character on the oxygen site. This provides a directly way to study the unoccupied e_g states to understand the electronic structure as well as the Mn-O bond. Here we will present a survey of the evolution of these states both as a function of composition and dimensionality (single layer to 3D perovskite). As the system transitions between ordered and disordered states (ferromagnetic metallic, charge ordered, anti-ferromagnetic insulating,...), we can view directly changes in the electronic structure to better understand the behavior of the manganites.

*Work at Argonne was supported by the U.S. Department of Energy, Office of Science, under Contract No. W-31-109-Eng-38.

Charge Ordering and Ferroelectricity in Oxides

Daniel Khomskii
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Charge ordering is quite common in transition metal oxides. It treating it one usually considers site-centered superstructures. Such are for instance the standard checkerboard charge ordering in $La_{0.5}Ca_{0.5}MnO_3$, or Verwey charge ordering in magnetite. However there exist another possibility: bond-centered superstructures, such as e.g. the Peierls state in low-dimensional systems. Especially interesting situation can appear if these two types of ordering coexist: this will naturally lead to the appearance of ferroelectricity in such systems. In this talk I will consider the possibility of competition or coexistence of site-centered and bond-centered structures on a few examples. One is the charge ordering in less-than-half-doped manganites. We have recently shown that in this case indeed a bond-centered ordering may exist, and, moreover, bond-centered ordering may coexist with site-centered one, in which case the resulting state would be ferroelectric. This as a rare case of ferroelectricity in magnetic material the so called multiferroic behaviour. I will consider some other systems in which the same phenomenon can take place. In particular insulating nickelates $RNiO_3$, especially with small rare earth R, show charge disproportionation into $Ni(3\delta)$, and with certain type of magnetic ordering these systems may also be multiferroic. And the most interesting such example may be magnetite Fe_3O_4 below the Verwey transition.

Competition of local and long-range polar order in relaxor ferroelectrics

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Neutron and x-ray diffraction have been used to study the competing local and long-range polar orders in the relaxor ferroelectrics $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN) and $Pb(Zn_{1/3}Nb_{2/3})O_3$ (PZN) under an electric field. The results from the two relaxor systems are distinctively different. In PZN, the field induces long-range polar order , without being able to suppress the (overall) local polar order, measured with diffuse scattering intensities. The structure (long-range order) and diffuse scattering (local order) both have a strong field memory effect, associated with ferroelectric domain formations. In PMN, the unit cell shape in the bulk volume remains cubic for E up to 8 kV/cm, while a clear suppression of the diffuse scattering and concomitant enhancement of the Bragg peak intensity is observed, indicating a more ordered structure with increasing E field. However, the absence of hysteresis of these changes suggests that the ground state is not a frozen glassy phase as previously postulated.

Recent Results on CMR and Multiferroic Manganese Oxides

J. W. Lynn

NIST Center for Neutron Research, NIST, Gaithersburg, MD 20899-8562

Recent neutron and x-ray scattering results will be presented on both multiferroic materials and CMR systems. For the multiferroics, we have been investigating the magnetic structure of hexagonal $HoMnO_3$ as a function of temperature and field., which is a commensurate antiferromagnetic (T_N=72 K) ferroelectric (T_C=875 K). Three different chiral symmetries describe the zero field magnetic phases, with strong dielectric anomalies associated with the phase transitions. The spin dynamics is well described by a Heisenberg model in two dimensions. Orthorhombic $TbMnO_3$ develops a longitudinally polarized spin density wave state below 41 K, with a change in magnetic structure at 28 K that permits the development of ferroelectricity, while the magnetic structure remains incommensurate. For the RMn_2O_5 system (R=Tb, Dy, Ho) strong anomalies in the specific heat, thermal expansion, and dielectric constant are a manifestation of the magnetism to the ferroelectricity. For the Kagome staircase system $Co_3V_2O_8$ the rich variety of magnetic phases and lock-in transitions is a signature of the competing interactions, and is quite different than ferroelectric $Ni_3V_2O_8$. For the CMR system, we will discuss recent results for the polaron dynamics in optimally doped (La-Ba)MnO_3 and (La-Sr)MnO_3, and compare these results with (La-Ca)MnO_3 and the bilayer manganite system.
Detailed information and publications are available at http://www.ncnr.nist.gov/staff/jeff/

The great impact of substitution upon the electrical and magnetic states of metal-transition perovskite oxides

V. Caignaert, V. Hardy, S. Hébert, A. Maignan, D. Pelloquin, V. Pralong
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Subtle changes of stoichiometry or small amounts of chemical substitutions in perovskite manganites are known to strongly change the physical properties of these transition metal oxides. In order to generalize these effects to other 3d/4d metals, several other examples will be shown such as : (i) the induced abrupt magnetization jumps observed at low T in the M(H) curves of CMR manganites $Ln_{1-x}A_xMnO_3$ (L = lanthanide, A = alkaline earths) substituted either at the Ln/A or Mn-sites, (ii) the large changes of either Seebeck coefficient, from positive to negative or magnetic state, from antiferro to ferromagnetism, in perovskites $Ln_{1-x}A_xCoO_{3-\delta}$, (iii) Cr^{3+}/Ti^{4+} substitutions in the ruthenates $SrRuO_3$ and $CaRuO_3$ reinforcing or inducing ferromagnetism, (iv) extension to other more complex structures such as thermoelectric misfit cobaltites/rhodates and "114", $LBaCo_4O_{7+\delta}$, phases. For the understanding of the Seebeck measurements, a special care will be given to the important role played by the spin states, in particular for the cobalt cations and the spin degeneracy term in the modified Heikes formula.

Spontaneous rotation of orbital stripes and ferroelectric state in bilayer manganites

Yusuke Tokunaga[1], Yunsang Lee[1], Reiji Kumai[2], Masaya Uchida[1], Thomas Lottermoser[1], Takahisa Arima[*1], Yoshinori Tokura[†1]

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Recently, a new type of ferroelectric states which are inherently originated in the charge-ordered phenomena have been reported for such as charge-frustrated mixed valence system $LuFe_2O_4$, and also theoretically predicted for manganites. Here we report on the novel charge-polarized state accompanied by the spontaneous rotation of orbital stripes in charge/orbital-ordered bilayer manganites.

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Multiferroic behavior in RMn_2O_5 materials (R=Y,Tb)

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I will review recent experimental studies of RMn_2O_5 materials by neutron diffraction. In particular, I will discuss a microscopic mechanism, based on magnetic exchange-striction, that explains how the complex spin arrangements (incommensurate spin density waves) found at low temperature can induce a ferroelectric state. I will also briefly discuss the symmetry constraints on the electrical polarization in materials with incommensurate magnetic order.

Structural and Magnetic Properties of the Extended Kagome Antiferromagnet $RBaCo_4O_7$ (R=Y,Yb,Tm,Lu)

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The mixed-valent Co^{3+}/Co^{4+} compound $RBaCo_4O_7$ (R=Y,Yb,Tm,Lu) is built up of Kagome sheets of CoO_4 tetrahedra linked in the third dimension by a triangular layer of CoO_4 tetrahedra in an analogous fashion to that found in the known geometrically frustrated magnets such as pyrochlores and $SrCr_{9x}Ga_{12-9x}O_{19}$. We have undertaken a study of the structural and magnetic properties of these compounds using combined high-resolution powder neutron and synchrotron x-ray diffraction. Here we identify the role of charge-order and structural transitions in breaking geometric frustration in favor of magnetic order. We also discuss how the unique antiferromagnetic structure of this compound reveals a competition between in-plane and out-of-plane interactions. We also discuss the sensitivity of properties to oxygen content and speculate on mechanisms to 're-frustrate' the magnetic interactions.

The true magnetic nature of CMR Cobaltites

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In this talk I will focus on recent neutron scattering measurements on single crystals of $La_{1-x}Sr_xCoO_3$ to discuss the nature of the magnetic state, how it changes with hole concentration and its implications to the electronic transport.

*Also at NIST

Dance of Electrons on a Triangular Lattice (Na_xCoO_2) *

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The essential framework for cuprate superconductivity is that of a spin-1/2 electron system in the vicinity of a half filled (Mott limit) lattice. Of all oxide superconductors this framework is most closely matched in the sodium cobalt oxides except that it is realized on a triangular lattice. Besides superconductivity, the system exhibits spin-thermopower, metal-insulator transition, spin-density-wave, charge-order and anti-ferromagnetism. Since its discovery in 2003, we have reported the first single Fermi surface with its hexagonal topology [1], determined the sign of single-particle hopping to be negative ruling out a few instabilities in the system, and found an unusual temperature dependence of the quasiparticle weight providing the basic foundation for the low-energy electronic structure of cobaltates [1]. These results significantly narrowed down the choices for the superconducting order parameters. In this talk, I plan to focus on some new intriguing behaviour obtained by studying recent high quality samples of the parent superconductor[3] and the unusual insulator in a nearby doping[4].

Reference: [1] M.Z. Hasan et.al., Phys. Rev. Lett. 92, 286402 (2004). [2] A. Kuprin et.al., JPCS 67, 235 (2006). [3] D. Qian et.al., Phys. Rev. Lett. 96, 216405 (2006). [4] D. Qian et.al., Phys. Rev. Lett. 96, 046407 (2006).

*This work is in collaboration with L. Wray, D. Hsieh, D. Wu, J. L. Luo, N. L. Wang, A. Kuprin, A. Fedorov, R. J. Cava, L. Viciu

Orbital Ordering in Layered Ruthenates

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X-ray scattering techniques were used to probe ordering of the Ru 4d orbitals in single-layer and bilayer ruthenates. In the former ($Ca_{2-x}Sr_xRuO_4$, $x \leq 0.1$), resonant x-ray scattering was used on APS beamline 4ID-D, and large resonant enhancements at the L_2 and L_3 edges (2p $\rightarrow$ 4d transitions) were observed. For x = 0 crystals, scattering at the magnetic ordering wavevector— but well above T_N— was observed, and exhibited a transition at a temperature of $\sim$260 K. Based on the temperature and polarization dependences of this additional scattering, as well as muon spin resonance results that show no measurable magnetic moment above T_N, it is indicative of 4d t_{2g} orbital ordering. Scattering consistent with the same orbital ordering structure was also observed in an x = 0.1 crystal.

In bilayer calcium ruthenate ($Ca_3Ru_2O_7$), the c-axis lattice parameter collapse was studied as a function of temperature and magnetic field using the 13 T, High-Field Facility at NSLS beamline X21. The <0.1% structural change coincides in zero field with a metal-insulator transition, and may signal the onset of orbital ordering. High-field measurements therefore enabled the coupling between the lattice and spin degrees of freedom to be investigated, and shed light on the proposed orbital ordering. In our studies, anisotropy of the structural change for magnetic field applied along different in-plane directions was observed, and is compared to published work based on resistivity, magnetization, and Raman scattering measurements.

Work performed in collaboration with J.P. Hill, S.C. LaMarra, I. Zegkinoglou, B. Bohnenbuck, J. Strempfer, J. Chakhalian, C. Bernhard, B. Keimer, J.C. Lang, G. Srajer, H. Fukazawa, S. Nakatsuji, Y. Maeno, R. Jin, D. Mandrus, S.I. Ikeda, Y. Yoshida, and N. Kikugawa.

Temperature Dependent Bilayer Ferromagnetism in $Sr_3Ru_2O_7$*

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The Ruthenium based perovskites exhibit a wide variety of interesting collective phenomena related to magnetism originating from the Ru 4d electrons. Much remains unknown concerning the nature of magnetic fluctuations and excitations in these systems. We present results of detailed inelastic neutron scattering measurements of $Sr_3Ru_2O_7$ as a function of temperature, probing the ferromagnetic fluctuations of the bilayer structure†. A magnetic response is clearly visible for a range of temperatures, $T = 3.8$ K up to $T = 100$ K, and for energy transfers between $\hbar\omega = 2$ meV and 14 meV. These measurements indicate that the ferromagnetic fluctuations manifest in the bilayer structure factor persist to surprisingly large temperatures. This behavior may be related to the proximity of the system in zero magnetic field to the metamagnetic/ferromagnetic transition.

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†M. B. Stone *et al.* Phys. Rev. B in press (2006)

Frustrated spinels under extreme conditions

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In this presentation, I will discuss the metastable states of frustrated spinels that are induced by an external magnetic field.

Spontenaous spin-lattice coupling in the geometrically frustrated triangular lattice antiferromagnet $CuFeO_2$

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$CuFeO_2$ is a geometrically frustrated triangular lattice antiferromagnet that has been shown to exhibit magnetoelectric behavior. We used high-resolution synchrotron X-ray and neutron diffraction to study the lattice and magnetic properties of this system in a magnetic field. On cooling from room temperature, $CuFeO_2$ undergoes two antiferromagnetic phase transitions with incommensurate and commensurate magnetic order at $T_{N1} = 14$ K and $T_{N2} = 11$ K, respectively. The occurrence of these two magnetic transitions is accompanied by second- and first-order structural phase transitions from a hexagonal to a monoclinic structure. Application of a 6.9 T magnetic field lowers both transition temperatures by approx. 1 K, and induces an additional incommensurate structural modulation in the temperature region where the field-driven ferroelectricity occurs. These results demonstrate the strong magneto-elastic coupling that is intimately related to the multiferroic effect