TT 43: Correlated Electrons: Metal-Insulator Transition 2

Time: Thursday 15:00–17:45 Location: H 3010

TT 43.1 Thu 15:00 H 3010

Correlation effects in ruthenates: LDA+DMFT study — •Evgeny Gorelov and Eva Pavarini — IAS-3, Forschungszentrum Jülich, 52425 Jülich

The ruthenates of the Ruddlesden-Popper family $A_{n+1}\mathrm{Ru}_n\mathrm{O}_{3n+1}$ where $A = (\mathrm{Sr}, \mathrm{Ca})$ are unique among transition-metal oxides, because the change of cation A and/or in the number n of RuO_2 layers leads to a variety of collective phenomena, ranging from multi-band Mott transitions to ferro- and meta-magnetism. To understand these systems, it is necessary to disentangle the effects of Coulomb repulsion in the $4d^4$ Ru shell from those of lattice distortions and chemistry. By using the LDA+DMFT approach, we show how such disentanglement explains the nature of the metal-insulator transition in single-layered Ca ruthenates [1] and the evolution of electronic structure in n-layered Sr ruthenates [2]. We use LDA+DMFT scheme based on the N-th Order Muffin-Tin Orbital approach and the weak-coupling CT-quantum Monte Carlo method as impurity solver. This method allows us to take into account the full rotationally-invariant Coulomb interaction, as well as full on-site self-energy matrix in orbital space with spin-orbit coupling. We discuss changes in effective mass and orbital polarization as a result of spin-flip processes and spin-orbit interaction.

[1] E. Gorelov et al., Phys. Rev. Lett. **104**, 226401 (2010).
[2] M. Malvestuto et al., Phys. Rev. B **83**, 165121 (2011).

TT 43.2 Thu 15:15 H 3010

Modeling the disordering of the cooperative Jahn-Teller distortion in $KCuF_3$ — •Joaquin Gabriel Miranda[1], Erik Koch[1], and Eva Pavarini[2] — [1]German Research School for Simulations Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich — [2]Institute for Advanced Simulation and JARA, Forschungszentrum Jülich, 52425 Jülich

We study the melting of the cooperative Jahn-Teller distortion. To properly describe this order-disorder transition we have to work with large real-space cells. For this we use a combination of first-principle calculations (LDA+U) and Monte Carlo (MC) simulation. First we determine the potential energy surface for displacements of the fluorine ions. Subtracting the long-ranged Coulomb terms lead to a short-ranged parametrization of the dynamical matrix for pairs of fluorine displacements. We then use the parametrized LDA+U energies as the input for Monte Carlo simulations of extended supercells to study the spacial range of the lattice ordering as a function of temperature.

TT 43.3 Thu 15:30 H 3010

Response of acoustic phonons to charge and orbital order in $LaSr_2Mn_2O_7$ — •Frank Weber[1,2], Stephan Rosenkranz[2], John-Paul Castellan[2], Ray Osborn[2], Hong Zheng[2], John F. Mitchell[2], Ying Chen[3,4], Songxue Chi[3,4], Jeffrey W. Lynn[3], and Dmitry Reznik[1,5] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, Karlsruhe, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne IL, USA — [3]NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg MD, USA — [4]Department of Materials Science and Engineering, University of Maryland, USA — [5]Department of Physics, University of Colorado, USA

The acoustic phonons in the 50% doped bilayer manganite $LaSr_2Mn_2O_7$ exhibiting CE type charge order were investigated using inelastic neutron scattering. At the onset of charge ordering, we observe an abrupt increase(decrease) of the energies(linewidths) of the transverse acoustic phonon along (110), which crosses the CE ordering wavevector. This effect is, however, not localized at the CE ordering wave vector, but is observed over an extended range of momentum transfers, for which the phonon energy is lower than 15 meV. These observations indicate a reduced electron-phonon coupling due to a partial removal of the Fermi surface and provide direct evidence for a link between electron-phonon coupling and charge order in manganites. However, the observed response is not consistent with a standard charge-density-wave mechanism, clearly showing that the transition is unconventional.

TT 43.4 Thu 15:45 H 3010

Hour-glass dispersion in overdoped single-layered manganites — •H. Ulbrich[1], P. Steffens[2], D. Lamago[3], Y. Sidis[3], and M. Braden[1] — [1]University of Cologne — [2]ILL, Grenoble, France — [3]LLB Saclay, France

The mechanism of the high-T_c superconductivity in the cuprates is still an unsolved problem in modern solid state physics. Stripe ordering may play an important role in the physics of high-T_c superconductors. Experimentally, observations of the spin-wave dispersion which forms a shape like an hour-glass have been taken as proof for stripe scenarios in the cuprates [1]. Stripe ordering can be observed in several transition-metal compounds. In manganites, additionally the e_g-orbitals on Mn^{3+} ions play a crucial role. A pattern for the ordering schema in overdoped manganites (x> $\frac{1}{2}$) has just been established [2]. We studied the single-layered systems $Re_{1-x}A_{1+x}\mathrm{MnO}_4$ (Re=Pr,Nd; A=Ca,Sr) with x=$\frac{2}{3}$. The position of the magnetic superstructure reflections of Mn^{4+} exhibits a fourfold pattern. Inelastic neutron data around the incommensurate magnetic satellites reveal an hour-glass like spin-wave dispersion, comparable to the cuprates and recently in cobaltates [1,3]. However, our dispersion in the $Pr_{0.33}Ca_{1.67}MnO_4$ compound, which exhibits a large correlation length of the magnetic order, showing a branch dispersing outward from the incommensurate zone-center. Upon heating, the correlation length decreases and concomitantly, the dispersion develops in a full hour-glass shape.

[1] J.M. Tranquada et al., Nature, 429, 534 (2004).
[2] H. Ulbrich et al., Phys. Rev. Lett. 106, 157201 (2011).
[3] A.T. Boothroyd et al., Nature 471, 341 (2011).

TT 43.5 Thu 16:00 H 3010

Signature of antiferromagnetic long range order in the optical spectrum of strongly correlated electron systems — •Ciro Taranto[1], Giorgio Sangiovanni[1], Antoine Georges[2,3,4], Massimo Capone[5], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France — [4]DPMC, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève, Suisse — [5]Democritos National Simulation Center, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali (IOM) and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, 34136 Trieste, Italy

We show how the onset of a non-slater antiferromagnetic ordering in a correlated material can be detected by optical spectroscopy. Using dynamical mean-field theory we identify [1] two distinct features: The antiferromagnetic ordering is associated with an enhanced spectral weight above the optical gap, and well separated spin-polaron peaks emerge in the optical spectrum. Both features are indeed observed in $LaSrMnO_4$[2].

[1]C. Taranto, G. Sangiovanni, A. Georges, M. Capone, K. Held and A. Toschi, *in preparation.*
[2]A. Gössling, M. W. Haverkort, M. Benomar, Hua Wu, D. Senff, T. Möller, M. Braden, J. A. Mydosh and M. Grüninger, Phys. Rev. B **77** , 035109 (2008).

15 min. break.

TT 43.6 Thu 16:30 H 3010

Orbital-order melting in rare-earth manganites — •Andreas Flesch[1], Guoren Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Institute for Advanced Simulation and JARA, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]German Research School for Simulation Sciences, 52425 Jülich, Germany

The mechanism of orbital ordering in rare-earth manganites, in particular in $LaMnO_3$, has been debated since long. For $LaMnO_3$, it was recently shown that the purely electronic super-exchange mechanism alone cannot explain the persistence of Jahn-Teller distortions in nanoclusters at high temperature [1]. However, its role in the orbital order-to-disorder transition (orbital-order melting) remains unclear. In this talk, we present order parameter (orbital polarization) and total energy calculations based on the LDA+DMFT approach for the series of rare-earth manganites. By comparing our results to experiments, we show that super-exchange plays a minor role in the orbital-order melting transition observed in rare-earth manganites [2].

[1] E. Pavarini and E. Koch, PRL **104**, 086402 (2010)

[2] A. Flesch, G. Zhang, E. Koch, and E. Pavarini, arXiv:1106.2439

TT 43.7 Thu 16:45 H 3010

Ultrafast strain engineering in complex oxide heterostructures — •Paul Popovich[1], Andrea Caviglia[1], Raoul Scherwitzl[3], Wanzheng Hu[1], Hubertus Bromberger[1], Rashmi Singla[1], Matteo Mitrano[1], Matthias C. Hoffmann[1], Stefan Kaiser[1], Pavlo Zubko[3], Sergio Gariglio[3], Jean-Marc Triscone[3], Michael Först[1], and Andrea Cavalleri[1,2] — [1]Max-Planck Research Group for Structural Dynamics - Center for Free Electron Laser Science, University of Hamburg, Germany — [2]Department of Physics, Clarendon Laboratory, University of Oxford, UK — [3]Departement de Physique de la Matiere Condensee, University of Geneva, 24 Quai Ernest-Ansermet, 1211 Geneve 4, Switzerland

The mechanical coupling between the substrate and the thin film is expected to be effective on the ultrafast timescale, and could be exploited for the dynamic control of materials properties. Here, we demonstrate that a large-amplitude mid-infrared field, made resonant with a stretching mode of the substrate, can switch the electronic properties of a thin film across an interface. Exploiting dynamic strain propagation between different components of a heterostructure, insulating antiferromagnetic $NdNiO_3$ is driven through a prompt, five-order-of-magnitude increase of the electrical conductivity, with resonant frequency and susceptibility that is controlled by choice of the substrate material. Vibrational phase control, extended here to a wide class of heterostructures and interfaces, may be conducive to new strategies for electronic phase control at THz repetition rates.

TT 43.8 Thu 17:00 H 3010

Coherent phonons: an all-optic probe of ultrafast structural phase transitions — •Laura Foglia[1], Simon Wall[1], Daniel Wegkamp[1], Kannatassen Appavoo[2], Joyeeta Nag[2], Richard F. Haglund[2], Julia Stähler[1], and Martin Wolf[1] — [1]Fritz-Haber-Institut der MPG, Dep. of Phys. Chem., Berlin, Germany — [2]Dep. of Physics and Astronomy, Vanderbilt University, Nashville, USA

The ionic equilibrium position in a crystal and its vibrational response to an external perturbation are determined by the lattice potential, resulting from the interaction of cores and electrons. During a structural phase transition, the lattice potential symmetry changes, modifying both ionic positions and phonon spectrum. If the transition is driven out of equilibrium, the potential may change on a different time scale than the ionic positions. We exploit the generation of coherent phonons by a laser pulse as an all-optical probe of the lattice potential symmetry with fs time resolution, and apply this technique to the study of the photoinduced phase transition in VO_2. Coherent phonons are observed as a modulation of the broadband transient reflectivity for fluences below the transition threshold $\Phi_c = 6.2\mathrm{mJ/cm}^2$. This modulation, due to the four lowest Raman active modes of the monoclinic VO_2 phase, disappears above Φ_c. By measuring the coherent response of the excited state in a three pulse experiment, we show that the change of the potential symmetry occurs on a sub-phonon-period time scale, much faster than the lattice rearrangement. We conclude that, in this non-equilibrium regime, the photoinduced phase transition is directly driven by electron-induced changes of the lattice potential.

TT 43.9 Thu 17:15 H 3010

An efficient treatment of the high-frequency tail of the self-energy function and its relevance for multi-orbital models — •Gang Li and Werner Hanke — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

An efficient and stable method is presented to determine the one-particle Green's function in the hybridization-expansion continuous-time (CT-HYB) Quantum Monte Carlo method, within the framework of dynamical mean-field theory. The high-frequency tail of the impurity self-energy is replaced by a noise-free function determined by a dual-expansion around the atomic limit. This scheme essentially does not depend on the explicit form of the interaction term and does not introduce additional numerical cost to the runtime simulation. As an application, a 2-orbital Anderson impurity model with a general on-site interaction form is studied. The phase diagram is extracted as a function of the Coulomb interactions for a varity of Hund's coupling strengths.

TT 43.10 Thu 17:30 H 3010

Effective models for spin liquid phases in Hubbard models — Hong Yu Yang[1], Fabrizio Albuquerque[2], Sylvain Capponi[2], Andreas Läuchli[3], and •Kai Phillip Schmidt[4] — [1]Institut de théorie des phénomènes physiques, EPF Lausanne, 1015 Lausanne, Switzerland — [2]Laboratoire de Physique Théorique, IRSAMC, Université Paul Sabatier, 31062 Toulouse Cedex 04, France — [3]Institut für Theoretische Physik, Universität Innsbruck, 6020 Innsbruck, Austria — [4]Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

The Hubbard model is one of the most studied microscopic models in condensed matter physics. It describes on a very simple level the interplay between the kinetics and the Coulomb interaction of electrons in solid state systems. Generically, one expects at half filling a metallic phase for large kinetics while a Mott insulator is present for large interactions. In recent years more and more evidences have been found that especially on frustrated lattices there is the possibility of exotic and insulating intermediate phases without long-range order. It is therefore an obviously relevant question what kind of effective low-energy theory describes such Mott phases and how to derive them. This is particular complicated when the spin liquid is located close to the metal-insulator transition as for the recently discovered spin liquid of the Hubbard model on the honeycomb lattice. In this talk we discuss these issues for the Mott phase of the Hubbard model on the triangular and on the honeycomb lattice.