

## TT 26: Metal-Insulator Transition

Time: Thursday 14:00–17:30

Location: H19

TT 26.1 Thu 14:00 H19

**Local correlations and hole doping in NiO** — ●JAN KUNES<sup>1</sup>, VLADIMIR I. ANISIMOV<sup>2</sup>, ALEXEY V. LUKOYANOV<sup>3</sup>, and DIETER VOLLHARDT<sup>1</sup> — <sup>1</sup>Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg 86135 — <sup>2</sup>Institute of Metal Physics, Russian Academy of Sciences - Ural Division, 620041 Yekaterinburg GSP-170, Russia — <sup>3</sup>Ural State Technical University - UPI, 620002 Yekaterinburg, Russia

Charge-transfer (CT) insulators present an important subgroup of transition metal compounds which exhibit phenomena such as metal-insulator transitions or high temperature superconductivity. The location of ligand states between the interaction-split d bands leads to additional complexity, which requires a description beyond a simple Hubbard model. Using a combination of ab initio bandstructure and dynamical mean field theory (DMFT) we study the prototypical CT insulator NiO. Including the ligand p orbitals to the effective Hamiltonian, we obtain good agreement with PES and IPES data. Further we investigate the effect of hole doping. We find the additional holes to occupy mainly the ligand p orbitals despite large Ni-d spectral weight at the top of the valence band. Moreover, heavy hole doping leads to a significant reconstruction of the single-particle spectrum and filling of the charge-transfer gap. This is the first LDA+DMFT study of charge transfer systems, which includes the p-d hybridization explicitly and is thus able to provide a full description of valence and conduction band spectra.

TT 26.2 Thu 14:15 H19

**Unusual magnetic ground state in MnO under pressure.** — ●KLAUS KOEPERNIK<sup>1</sup>, DEEPA KASINATHAN<sup>2</sup>, and WARREN E. PICKETT<sup>3</sup> — <sup>1</sup>IFW Dresden, Germany — <sup>2</sup>MPI-CPFS Dresden, Germany — <sup>3</sup>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 5/2 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-orbital exchange terms. The dependence of the results on the parameters U and J will be discussed.

TT 26.3 Thu 14:30 H19

**Pressure-induced deconfinement and structural phase transition in the quasi-1D Bechgaard-Fabre salts** — ●A. PASHKIN<sup>1</sup>, M. DRESSEL<sup>2</sup>, and C. A. KUNTSCHER<sup>1</sup> — <sup>1</sup>Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — <sup>2</sup>1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

We have performed pressure-dependent x-ray diffraction and infrared spectroscopic studies of the organic low-dimensional conductors (TMTTF)<sub>2</sub>PF<sub>6</sub> and (TMTSF)<sub>2</sub>PF<sub>6</sub>, which belong to the family of the Bechgaard-Fabre salts. The (TMTTF)<sub>2</sub>PF<sub>6</sub> salt consists of basically uncoupled molecular stacks (half-filled) and is a prime example of a one-dimensional Mott-Hubbard insulator. On the other hand, the coupling between the stacks in the (TMTSF)<sub>2</sub>PF<sub>6</sub> salt is high enough to induce metallic conductivity, which is particularly pronounced along the stacking direction. The application of external pressure increases the interstack hopping in the Bechgaard-Fabre salts and allows for a continuous tuning of their electronic properties.

Our pressure-dependent x-ray diffraction data evidence a structural phase transition in (TMTTF)<sub>2</sub>PF<sub>6</sub> and (TMTSF)<sub>2</sub>PF<sub>6</sub> salts at about 5 and 8 GPa, respectively. Furthermore, we found a pressure-induced deconfinement transition from a one-dimensional Mott-Hubbard insulating state to a higher dimensional metallic state in (TMTTF)<sub>2</sub>PF<sub>6</sub> at about 2 GPa. The possible influence of the pressure-induced structural phase transition on the electronic properties is also discussed.

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TT 26.4 Thu 14:45 H19

**Valence, spin and orbital states of the quasi-one-dimensional**

**Ca<sub>3</sub>CoRhO<sub>6</sub>: band structure calculations and x-ray absorption spectroscopy study** — ●HUA WU, ZHIWEI HU, TOBIAS BURNUS, DANIEL KHOMSKII, and LIU HAO TJENG — II. Physikalisches Institut, Universität zu Köln, Zùlpicher Straße 77, 50937 Köln

Quasi-one-dimensional cobaltate Ca<sub>3</sub>Co<sub>2</sub>O<sub>6</sub> [1,2] and its isostructural Ca<sub>3</sub>CoRhO<sub>6</sub> have drawn attention recently due to the peculiar crystal structure and the fascinating magnetic properties. The valence (and orbital) state issue and the origin of the intra-chain Ising ferromagnetism remain unresolved for Ca<sub>3</sub>CoRhO<sub>6</sub>. Taking the insulating state of this material as a key finding, we applied the density-functional theory plus Hubbard U (DFT+U) method to study its electronic structure. We find that Ca<sub>3</sub>CoRhO<sub>6</sub> has the high-spin Co<sup>2+</sup> and low-spin Rh<sup>4+</sup>, and that it is the spin-orbit coupling which lifts the Co<sup>2+</sup> orbital degeneracy, thereby enabling the DFT+U to generate the band gap. We predict that the Co<sup>2+</sup> ion has a huge orbital magnetic moment of 1.7μ<sub>B</sub>, which accounts for the Ising magnetism. We also propose a model to explain the intra-chain ferromagnetism. Those results are confirmed by our x-ray absorption spectroscopy and x-ray magnetic circular dichroism study.

[1] Hua Wu, M. W. Haverkort, Z. Hu, D. I. Khomskii, and L. H. Tjeng, Phys. Rev. Lett. **95**, 186401 (2005).

[2] T. Burnus, Z. Hu, M. W. Haverkort, J. C. Cezar, D. Flahaut, V. Hardy, A. Maignan, N. B. Brookes, A. Tanaka, H. H. Hsieh, H.-J. Lin, C. T. Chen, and L. H. Tjeng, Phys. Rev. B **74**, 245111 (2006).

TT 26.5 Thu 15:00 H19

**Lattice response at the Mott Transition in a Quasi-2D Organic Conductor** — ●MARIANO DE SOUZA<sup>1</sup>, ANDREAS BRÜHL<sup>1</sup>, CHRISTIAN STRACK<sup>1</sup>, BERND WOLF<sup>1</sup>, DIETER SCHWEITZER<sup>2</sup>, and MICHAEL LANG<sup>1</sup> — <sup>1</sup>Physikalisches Institut, J. W. Goethe-Universität, Frankfurt am Main — <sup>2</sup>3. Physikalisches Institut, Universität Stuttgart, Stuttgart

The Mott transition, which is the metal-insulator (MI) transition driven by electron-electron interactions, is one of the key topics of research in the field of strongly correlated electron systems. Deuterated salts of the organic κ-(BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Br charge-transfer salts, here BEDT-TTF (or simply ET) denotes the donor molecule bis(ethylenedithio)tetrathiafulvalene and X a monovalent anion, have been recently discussed in this context. In this contribution we report on the direct observation of the lattice response through the Mott transition in the above-mentioned compound. Discontinuous changes of the lattice parameters at the Mott transition are detected by high-resolution dilatometry experiments. The uniaxial expansivities uncover a striking and unexpected anisotropy. A second-order phase transition is observed near the end-point of the first-order transition line T<sub>MI</sub>. The extraordinarily large lattice response there provides a sensitive thermodynamic probe to explore the critical behavior. The analysis yields a singular contribution with a critical exponent  $\tilde{\alpha} = 0.6 \sim 0.9$  and indicates the particular role of inhomogeneities giving rise to a broadening of the transition.

TT 26.6 Thu 15:15 H19

**Electron-Phonon Interaction and Antiferromagnetic Correlations** — ●GIORGIO SANGIOVANNI<sup>1</sup>, OLLE GUNNARSSON<sup>1</sup>, ERIK KOCH<sup>2</sup>, CLAUDIO CASTELLANI<sup>3</sup>, and MASSIMO CAPONE<sup>3,4</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Stuttgart — <sup>2</sup>Institut für Festkörperforschung, Jülich — <sup>3</sup>University of Rome "La Sapienza", Rome, Italy — <sup>4</sup>INFN-SMC and Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, 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.

TT 26.7 Thu 15:30 H19

**Spin wave dispersion in the helical spin ordered system SrFeO<sub>3</sub> and CaFeO<sub>3</sub>** — ●C. ULRICH<sup>1</sup>, M. REEHUIS<sup>1,2</sup>, G. KHALIULLIN<sup>1</sup>, V. DAMLJANOVIC<sup>1</sup>, A. MALJUK<sup>1,2</sup>, A. IVANOV<sup>3</sup>, K. SCHMALZL<sup>3</sup>, CH. NIEDERMAYER<sup>4</sup>, K. HRADIL<sup>5</sup>, A. SCHNEIDEWIND<sup>5</sup>, and B. KEIMER<sup>1</sup> — <sup>1</sup>Max-Planck-Institut FKF, Stuttgart, Germany — <sup>2</sup>Hahn-Meitner-Institut, Berlin, Germany — <sup>3</sup>Institut Laue-Langevin, Grenoble, France — <sup>4</sup>Paul-Scherrer-Institut, Villigen, Switzerland — <sup>5</sup>FRM II, München, Germany

One of the most interesting problems in condensed matter physics is the metal-insulator (MI) transition driven by strong electron correlations. The cubic perovskites SrFeO<sub>3</sub> and CaFeO<sub>3</sub> are isoelectronic to the manganite system and exhibit also colossal magneto resistance effects. But in contrast, the ferrates show a helical instead of a collinear spin structure. Furthermore, perfectly cubic SrFeO<sub>3</sub> shows no charge order and is metallic whereas pseudocubic CaFeO<sub>3</sub> shows a MI-transition at the charge ordering transition of 290 K. Therefore, both compounds are right at the borderline between itinerant and strongly correlated electron systems. We have determined the static and dynamic spin properties by neutron scattering. The extracted parameters in the spin Hamiltonian are a big step towards the understanding of the mechanisms behind the helical spin order and the charge order in the ferrates.

15 min. break

TT 26.8 Thu 16:00 H19

**Orbitally selective Mott transition in the two-band Hubbard model** — ●THEODOULOS COSTI and ANSGAR LIEBSCH — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

The two-band Hubbard model with inequivalent bands exhibits as a function of increasing local Coulomb repulsion two, in general quite different, "Mott" transitions at Coulomb interactions  $U_{c1}$  and  $U_{c2}$  respectively. We use the numerical renormalization group and exact diagonalization methods to investigate the nature of the second "Mott" transition in detail, for isotropic and anisotropic Hund's exchange [1]. The numerical renormalization group approach uses an effective low energy model which is valid for Coulomb interactions  $U > U_{c1}$ . We show that this model exhibits non-Fermi liquid and bad metallic behavior in the orbitally selective Mott phases for isotropic and anisotropic Hund's exchange coupling, respectively.

[1] A. Liebsch and T. A. Costi, Eur. Phys. J. B51, 523 (2006)

TT 26.9 Thu 16:15 H19

**Orbital-ordering and phase transitions in the Mott insulators LaVO<sub>3</sub> and YVO<sub>3</sub>** — ●EVA PAVARINI<sup>1</sup>, MOLLY RAYCHAUDHURY<sup>2</sup>, and OLE ANDERSEN<sup>3</sup> — <sup>1</sup>Institut fuer Festkoerperforschung, Forschungszentrum Juelich, D-52425 Juelich, Germany — <sup>2</sup>S.N. Bose National Centre for Basic Sciences, Kolkata, India — <sup>3</sup>Max-Planck-Institut fuer Festkoerperforschung, Stuttgart, Germany

We calculate the electronic structure of the Mott insulating 3d<sup>2</sup> perovskites LaVO<sub>3</sub> and YVO<sub>3</sub>. Using the first-principles NMTO downfolding method we construct a low energy Hubbard Hamiltonian for the 3d  $t_{2g}$  bands; we solve this model by using dynamical mean-field theory. The calculated Hubbard bands and Mott gaps are in very good agreement with experimental spectroscopy data. We show that, while in YVO<sub>3</sub> orbital fluctuations are already suppressed at room temperature, in LaVO<sub>3</sub> this happens only in the low temperature monoclinic phase. In the low-temperature orbitally-ordered phases both the Jahn-Teller deformations of the VO<sub>6</sub> and the covalent interaction between the empty La (Y) d orbitals and the occupied V  $t_{2g}$  orbital concur to determine the type of orbital-ordering.

TT 26.10 Thu 16:30 H19

**Spin Peierls Instability, Bond Formation and Orbital Ordering in MgTi<sub>2</sub>O<sub>4</sub>** — ●STEFANO LEONI, LUIS CRACO, MIRIAM SCHMITT, and HELGE ROSNER — MPI CPfS, Dresden, Germany

The spinel titanate MgTi<sub>2</sub>O<sub>4</sub> undergoes a metal-insulator transition on cooling below  $T_c = 270$  K, with a symmetry lowering from cubic to tetragonal and a collective mutual rotation of the TiO<sub>6</sub> octahedra. This is accompanied by a reorganization of the bonding pattern, which results in bond formation and bond elongation in distinct directions. Also in this titanate, electronic correlation effects, structural distortions and bond breaking pattern are intertwined and concur to determine the physics of the system. Here we present an electronic structure study of the metal-insulator transition, showing that the latter can be nicely captured by an LDA+U approach. Furthermore, we

demonstrate the first order character of the transition, that reflects a complex pattern of bond formation and bond breaking, which modifies the Ti-Ti  $d-d$  hopping contributions. In our calculations the onsite-potential  $U$  works as a source of local asymmetry at the titanium sites. Along this line, structural distortions and electronic correlation effects can be decoupled, allowing for a closer elucidation of the symmetry lifting across the transition. This in turn allows to follow the onset of orbital ordering from a situation of full degeneracy to a reorganized structures, with changed bond formation.

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TT 26.11 Thu 16:45 H19

**$t_{2g}$  orbital order in magnetite** — ●C. F. CHANG<sup>1</sup>, C. SCHÜSSLER-LANGEHEINE<sup>1</sup>, J. SCHLAPPA<sup>1</sup>, H. OTT<sup>1</sup>, M. W. HAVERKORT<sup>1</sup>, M. BUCHHOLZ<sup>1</sup>, Z. HU<sup>1</sup>, A. TANAKA<sup>2</sup>, D. SCHMITZ<sup>3</sup>, E. SCHIERLE<sup>4</sup>, E. WESCHKE<sup>4</sup>, G. KAINDL<sup>4</sup>, and L. H. TJENG<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln — <sup>2</sup>ADSM, Hiroshima University — <sup>3</sup>HMI c/o BESSY — <sup>4</sup>Institut für Experimentalphysik, Freie Universität Berlin

The electronic structure of the low-temperature phase of magnetite (Fe<sub>3</sub>O<sub>4</sub>) has been a puzzle for many decades. Recent resonant soft diffraction experiments provided first direct evidence for charge order in this system. Using resonant soft x-ray diffraction at the Fe  $L_{2,3}$  resonance we found further evidence for orbital order in this system, which can be recognized from a pronounced polarization dependence of the scattered signal. Due to the cubic-to-monoclinic phase transition in magnetite, the low temperature phase usually consists of multiple twins with different crystalline orientations, which leads to ambiguities in the quantitative analysis of the polarization dependence. By applying epitaxial strain and weak magnetic fields to a thin film of magnetite we are able to reduce the number of crystalline twins in the low temperature phase. With the set of spectra taken from this partially un-twinned sample, a quantitative analysis of the character of orbital-order in magnetite becomes feasible. Supported by the DFG through SFB 608.

TT 26.12 Thu 17:00 H19

**X-ray magnetic circular dichroism study of LaMn<sub>0.5</sub>Co<sub>0.5</sub>O<sub>3</sub>** — ●T. BURNUS<sup>1</sup>, Z. HU<sup>1</sup>, H. H. HSIEH<sup>2</sup>, H.-J. LIN<sup>3</sup>, C.-T. CHEN<sup>3</sup>, P. A. JOY<sup>4</sup>, and L. H. TJENG<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Zùlpicher Straße 77, 50937 Köln — <sup>2</sup>Chung Cheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan — <sup>3</sup>National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30076, Taiwan — <sup>4</sup>Physical and Material Chemistry Division, National Chemical Laboratory, Pune 411008, India

The perovskite LaMn<sub>1-x</sub>Co<sub>x</sub>O<sub>3</sub> system shows a multitude of magnetic properties, ranging from the diamagnetic LaCoO<sub>3</sub> via ferromagnetism in the mixed region to the antiferromagnetic LaMnO<sub>3</sub>. For  $x = 0.5$  soft-X-ray absorption spectroscopy at the Co- $L_{3,2}$  and Mn- $L_{3,2}$  edge reveals the divalent state for cobalt ions and the tetravalent for manganese ions. X-ray magnetic circular dichroic (XMCD) spectra indicate ferromagnetic coupling between Co<sup>2+</sup> ions and Mn<sup>4+</sup> ions. We found from the analysis of the XMCD spectra using configuration-interaction cluster calculations that the orbital moment ( $L_z$ ) of Co<sup>2+</sup> is very sensitive to tetrahedral distortions of the CoO<sub>6</sub> octahedron.  $\langle L_z \rangle$  is close to 1 for the undistorted CoO<sub>6</sub> octahedron and becomes smaller or larger than 1 for elongated or compressed octahedra, respectively.

TT 26.13 Thu 17:15 H19

**Unexpected line shapes and Cross Section Effects in Hard X-ray Photoelectron Spectroscopy of transition metal oxides** —

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The recent progress in Hard X-ray Photoelectron Spectroscopy (HXPES) has facilitated access to bulk sensitive spectroscopic information that was previously unavailable. The large kinetic energies of photoelectrons in HXPES yield inelastic mean free paths of the order of 100 Å, thus providing essentially bulk sensitive results. In this respect, HXPES is an important improvement over standard photoemission in the soft x-ray or UV range having considerable surface contribution to the spectra. For correlated systems, this surface sensitivity is particularly problematic due to the possibly strong modifications of the electronic structure at the surface of these systems. We have investigated a number of simple transition metal (TM) oxides in order to

study the effects of variations in the photoionization cross sections for high photon energy spectra. We find that the line shapes of the valence band spectra are strongly modified as compared to lower photon energy results. In particular, we observe strongly enhanced contribu-

tions of the TM 4s which are two orders of magnitude more intense than in the soft x-ray regime. These results are of importance for the conception and interpretation of HXPES in correlated systems.