TT 9: Correlated Electrons: Metal-Insulator Transition 1

Time: Monday 14:00–16:45   Location: HSZ 03

TT 9.1   Mon 14:00   HSZ 03

Pressure and doping driven metal-to-insulator transition in V_2O_3 — •Philipp Hansmann[1,2], Alessandro Toschi[2], Giorgio Sangiovanni[2], Maurits Haverkort[1], Tanusri Saha-Dasgupta[3], and Karsten Held[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Solid State Physics, Vienna University of Technology, Austria — [3]S.N. Bose National Centre for Basic Sciences, Kolkata, India

In the V_2O_3 system chemical doping and application of pressure are usually assumed to have equivalent effects for the physics of the Mott Hubbard metal-to-insulator transition (MIT). Recent experimental evidence, however, shows that application of pressure on the Cr-doped V_2O_3 cannot repristinate the situation of the undoped compound. In order to understand the underlying physical mechanisms in the differently driven MITs we investigate optical and X-ray absorption spectra by means of the local density approximation and its merger with dynamical mean field theory (LDA+DMFT) as well as full multiplet cluster calculations.

TT 9.2   Mon 14:15   HSZ 03

Correlation effects in half-metallic Heusler alloys — •Eberhard Jakobi, Nils Blümer, and Peter van Dongen — KOMET337, Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland

Spintronic applications such as giant magnetoresistive or spin valve devices require materials with high spin polarization, ideally half metals at room temperature. Heusler alloys are an important class of candidates for such spintronic materials [1].

For these moderately correlated materials, density functional theory (DFT) appears as a reasonable starting point [2]. However, this description lacks lifetime effects and cannot exhibit Mott transitions.

We present results within dynamical mean-field theory (DMFT), obtained using a second-order weak-coupling impurity solver, which is optimized for treating systems with a large number of valence bands. Correlation effects lead to significant changes in the band-selective densities of states and to corrections in the local moments.
[1] Wurmehl et al, Appl. Phys. Lett. 88 (2006) 032503
[2] Kandpal et al, J. Phys. D: Appl. Phys. 40 (2007) 1507

TT 9.3   Mon 14:30   HSZ 03

LDA+DMFT study of metal-insulator transition in the bulk and at the surface of $Ca_xSr_{2-x}RuO_4$ — •Michael Karolak, Tim Wehling, Frank Lechermann, and Alexander Lichtenstein — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg

$Ca_xSr_{2-x}RuO_4$ is an interesting model system to study the interplay of structural distortions and the electronic metal to insulator transition. We present an ab-initio study within the LDA+DMFT framework of this system. In this way we account for changes in the one particle Hamiltonian due to the structural distortions in a first principles manner. We obtain the electronic density of states and the self energy. The mechanism of the metal to insulator transition in the bulk and at the surface of this system is discussed. A strong enhancement of electron correlation effects is found for the low temperature structures.

TT 9.4   Mon 14:45   HSZ 03

LDA+DMFT study of Ca_2RuO_4 and Sr_2RuO_4 using the full on-site Coulomb interaction — •Evgeny Gorelov[1], Eva Pavarini[1], and Alexander I. Lichtenstein[2] — [1]Forschungszentrum Jülich, IFF, 52425 Jülich, Germany — [2]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany

The $Ca_{2-x}Sr_xRuO_4$ layered ruthenates display a complex phase diagram. Whereas Sr_2RuO_4 is a correlated metal, the progressive substitution Sr with Ca leads to a number of structural phase changes. Finally, Ca_2RuO_4 exhibits Mott transition at T≈350 K [1].

In this work we calculate the photoemission spectra of Sr_2RuO_4 [2] and study the temperature-induced Mott transition in Ca_2RuO_4 [3].

As a method we use the LDA+DMFT technique. First we construct a material-specific NMTO Wannier basis for the partially filled 4d t_{2g} bands and the corresponding three-band t_{2g} Hubbard Hamiltonian. Then we solve this model within the DMFT approximation retaining the full self-energy matrix and using the Continuous Time QMC im-

purity solver [4]. This solver allow us to analyze the role played by the spin-flip terms of the on-site Coulomb vertex.
[1] O. Friedt, M. Braden, G. Andre, P. Adelmann, S. Nakatsuji, Y. Maeno, Phys. Rev. B **63**, 174432 (2001).
[2] E. Gorelov, A. N. Rubtsov, A.V. Lukoyanov, V.I. Anisimov and A. I. Lichtenstein, to be published.
[3] E. Gorelov and E. Pavarini, to be published.
[4] A. N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein, Phys. Rev. B **72**, 035122 (2005).

TT 9.5   Mon 15:00   HSZ 03

Drastic Spectral Weight Transfer across the Metal-Insulator Transition in $Ca_{2-x}Sr_xRuO_4$ Revealed by Soft-X-ray Photoemission — •H. Fujiwara[1], Z. Hu[1], T. C. Koethe[1], A. Hendricks[1], M. Zell[1], N. B. Brookes[2], S. Nakatsuji[3], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan

The layered $Ca_{2-x}Sr_xRuO_4$ system shows a very rich phase diagram as a function of the x-composition, temperature and magnetic field. Particularly fascinating is the electronic structure in the range of $0 < x < 0.2$ where the metal-insulator transition (MIT) takes place at a continuously decreasing temperature with x getting closer to 0.2. This transition is accompanied by a drop in the resistivity of several orders of magnitude, comparable to that in V_2O_3 and VO_2. In order to reveal the mechanism of the MIT in $Ca_{2-x}Sr_xRuO_4$, we have carried out a photoemission study with $h\nu = 700$ eV to obtain reasonable sensitivity to the Ru 4d spectral weight. We have found that there is a dramatic transfer of the spectral weight across the MIT. Since x-ray absorption spectroscopy has shown that the orbital occupation of the three t_{2g} bands changes significantly across the MIT, as is the case also in the MITs of V_2O_3 [1] and VO_2 [2], our results suggest the crucial role of the orbital switching for the MIT of $Ca_{2-x}Sr_xRuO_4$.
[1] J.-H. Park, et al., Phys. Rev. B 61, 11506 (2000).
[2] M. W. Haverkort, et al., Phys. Rev. Lett. 95, 196404 (2005).

15 min. break

TT 9.6   Mon 15:30   HSZ 03

Electronic and optical properties of NiS_2 — •Cosima Schuster — Universität Augsburg, D-86135 Augsburg

Crystal field splitting, correlation, and the 3d band width are almost equal in the pyrites MX_2 (M=Fe,Co,Ni; X=S,Se) which gives rise to a large variety of electrical, magnetic and optical properties in these compounds. Of special interest is the metal-insulator-transition in NiS_2 with Se-doping or by applied pressure. It is not accompanied by a change in the lattice symmetry and commonly believed to be driven by electron-electron interactions. In addition, a low-temperature antiferromagnetic phase is observed both in the insulating and metallic regime. To reinvestigate the properties of NiS_2 we perform ab initio calculations using density functional theory. Thereby we focus on the relation between doping and applied pressure and the role of the magnetism in the metal-insulator-transition. The magnetic phase diagram with pressure and doping can be reproduced within the GGA, albeit the magnetic phase is slightly overestimated. The insulating behaviour of NiS_2, however, cannot be described within this approximation. The description in terms of a gap and of the metal-insulator-transition and the optical properties near the transition need more advanced methods. The response functions obtained in the random phase approximation cannot sufficiently describe the optical properties.

TT 9.7   Mon 15:45   HSZ 03

Is NiS_2 a charge-transfer insulator? — •Jan Kuneš[1], Dmitry A Korotin[2], and Vladimir I Anisimov[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Institute of Metal Physics, Russian Academy of Sciences, Yekaterinburg, Russia

The physics NiS_2 and $NiSe_2$ is often described in terms of small respectively negative gap charge-transfer insulator. Using combination of first principles bandstructure and dynamical mean-field approximation, so called LDA+DMFT approach, we investigate the electronic structures of the two materials at ambient conditions and under pres-

sure. While both compounds are similar to charge-transfer insulators in that the ligand p-band is located between the Ni-d lower and upper Hubbard bands, the quasiparticle gap is not of the charge-transfer type. The gap is between a strongly hybridized $p - d$ valence band and a conduction band formed by anti-bonding states of S-S dimer with strong admixture of Ni-d character. The key difference between NiS_2 and $NiSe_2$ determining their groundstates is the stronger dimer splitting in the former.

TT 9.8   Mon 16:00   HSZ 03

Crystal-field level inversion in lightly Mn-doped $Sr_3Ru_2O_7$ — Muhammed A. Hossain[1], Zhiwei Hu[2], Maurits W. Haverkort[2], •Tobias Burnus[2], Chun Fu Chang[2], Stefan Klein[2], Jonathan D. Denlinger[3], Hong-Ji Lin[4], Chien Te Chen[4], Roland Mathieu[5], Y. Kaneko[5], Yoshinori Tokura[5], S. Satow[5], Y. Yoshida[6], Hidenori Takagi[5], Arata Tanaka[7], Ilya S. Elfimov[1], George A. Sawatzky[1], L. Hao Tjeng[2], and Andrea Damascelli[1] — [1]University of British Columbia, Vancouver, Canada — [2]II. Physikalisches Institut, Universität zu Köln — [3]Advanced Light Souce, Berkeley, California — [4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [5]University of Tokyo, Japan — [6]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan — [7]Hiroshima University, Japan

$Sr_3(Ru_{1-x}Mn_x)_2O_7$, in which $4d$-Ru is substituted by the more localized $3d$-Mn, is studied by x-ray dichroism and spin-resolved density functional theory. We find that Mn impurities do not exhibit the same 4+ valence of Ru, but act as 3+ acceptors; the extra e_g electron occupies the in-plane $3d_{x^2-y^2}$ orbital instead of the expected out-of-plane $3d_{3z^2-r^2}$. We propose that the $3d$–$4d$ interplay, via the ligand oxygen orbitals, is responsible for this crystal-field level inversion and the material's transition to an antiferromagnetic, possibly orbitally ordered, low-temperature state.

TT 9.9   Mon 16:15   HSZ 03

On the mechanism for orbital-ordering in $KCuF_3$ — •Eva Pavarini[1], Erik Koch[1], and Alexander I. Lichtenstein[2] — [1]Institut für Festkörperforschung and Institute for Advanced Simulations, Forschungzentrum Juelich — [2]Institute of Theoretical Physics, University of Hamburg

The Mott insulating perovskite $KCuF_3$ is considered the archetype of an orbitally-ordered system. By using the LDA+dynamical mean-field theory (DMFT) method, we investigate the mechanism for orbital-ordering (OO) in this material. We show that the purely electronic Kugel-Khomskii super-exchange mechanism (KK) alone leads to a remarkably large transition temperature of $T_{KK} \sim 350$ K. However, orbital-order is experimentally believed to persist to at least 800 K. Thus Jahn-Teller distortions are essential for stabilizing orbital-order at such high temperatures.

TT 9.10   Mon 16:30   HSZ 03

Predicting pressure-induced phase transitions in the Mott insulator TiOCl — Yuzhong Zhang, •Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

The layered Mott insulator TiOCl has been the focus of a lot of recent experimental and theoretical research as it is one of the few inorganic spin-Peierls materials. Still, several important issues remain unsettled, namely the underlying Hamiltonian, the mechanism that is responsible for the incommensurate phase and the nature of the high-pressure phases. We performed thorough density functional theory calculations in order to shed light on these issues. First, we determine the parameters of a very general spin-phonon Hamiltonian[1]. The resulting model for TiOCl has strong antiferromagnetic exchange couplings along one direction with weak but significant frustrating ferromagnetic couplings along the other two directions, and it has strong spin-lattice coupling constants. Using constant pressure Car Parrinello molecular dynamics calculations, we determine the high pressure structures of TiOCl from first principles[2]. We predict two consecutive phase transitions, first from a Mott insulating high symmetry structure to a metallic dimerized structure and then back to a metallic high symmetry structure. The first of the two transitions has since been confirmed by experiment.
[1] Y. Z. Zhang, H. O. Jeschke, and R. Valentí, Phys. Rev. B **78**, 205104 (2008).
[2] Y. Z. Zhang, H. O. Jeschke, and R. Valentí, Phys. Rev. Lett. **101**, 136406 (2008).