TT 31 Correlated Electrons: Metal Insulator Transition - Part 2

Time: Thursday 14:00–18:30 Room: HSZ 301

TT 31.1 Thu 14:00 HSZ 301

The spin states of $LaCoO_3$; a revision revised — •M. W. Haverkort[1], Z. Hu[1], J. C. Cezar[2], H. Wu[1], J. Gegner[1], T. Burnus[1], T. Koethe[1], H. Hartmann[1], M. Reuther[1], T. Lorenz[1], A. Tanaka[3], N. B. Brookes[2], H. H. Hsieh[4], H.-J. Lin[5], C. T. Chen[5], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]European Synchrotron Radiation Facility, Boîte Postale 220, 38043 Grenoble Cédex, France — [3]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan — [4]Chung Cheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan — [5]National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30076, Taiwan

Using soft x-ray absorption spectroscopy and magnetic circular dichroism at the Co-$L_{2,3}$ edge we show that the spin state transition in $LaCoO_3$ can be well described by a low-spin ground state and a high-spin first excited state which becomes populated at elevated temperatures. Sum rules used on the magnetic circular dichroism signal reveal a large orbital momentum, in good agreement with a low-/high-spin scenario, but hard to reconcile with a low-/intermediate-spin picture. We discuss why the original prediction of the intermediate-spin state from band theory may be questionable.

TT 31.2 Thu 14:15 HSZ 301

Electronic structure of $LaTiO_3$ and $YTiO_3$ — •A. Gössling[1], R. Rückamp[1], H. Roth[1], T. Lorenz[1], A. Freimuth[1], and M. Grüninger[2] — [1]II. Phys. Institute, University of Cologne, Germany — [2]II. Phys. Institute, University of Aachen, Germany

In Mott-Hubbard insulators, excitations from the lower to the upper Hubbard bands give rise to an interesting multi-peak structure in the optical conductivity. The spectral weight of these features is very sensitive to magnetic and orbital correlations.

Using spectroscopic ellipsometry, we determined the optical conductivity σ between 0.8 and 6 eV of the Mott-Hubbard insulators $YTiO_3$ and $LaTiO_3$ as function of temperature. While the spectra of $YTiO_3$ show a sizeable redistribution of spectral weight with temperature, those of $LaTiO_3$ are almost temperature independent. In $YTiO_3$ a strong anisotropy between $\sigma_{a,b}$ and σ_c is observed, which we trace back to an orbitally-ordered ground state.

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TT 31.3 Thu 14:30 HSZ 301

Raman light-scattering in the Mott-insulators $LaTiO_3$ and $YTiO_3$: Evidence for orbital excitations — •C. Ulrich[1], A. Gössling[2], M. Grüninger[3], M. Guennou[1], H. Roth[2], M. Cwik[2], T. Lorenz[2], G. Khaliullin[1], and B. Keimer[1] — [1]Max-Planck-Institut FKF, Stuttgart — [2]Universität zu Köln — [3]RWTH Universität Aachen

Collective excitations of the valence electrons between different atomic orbitals (termed "orbitons") contain a wealth of information about the different types of interactions between the spin, charge and orbital arrangement of the electrons. Experiments introducing Raman scattering as a direct probe of orbitons in $LaMnO_3$ [1] have hence opened up new perspectives. However, the results have proven to be quite controversial [2,3]. In order to identify orbital excitations in the titanates $LaTiO_3$ and $YTiO_3$ we have used the Raman light scattering technique. The Raman spectrum of these Mott-insulators exhibits pronounced electronic excitations around 230 meV, i.e. well above the energy range of two-phonon excitations. Based on the temperature, polarization, and photon energy dependence, this mode is identified as orbital excitation. The observed profiles bear a striking resemblance to magnetic Raman modes in the insulating parent compounds of the superconducting cuprates, indicating an unanticipated universality of the electronic excitations in transition metal oxides. [1] E. Saitoh et al., Nature 410, 180 (2001). [2] M. Grüninger et al., Nature 418, 39 (2002). [3] E. Saitoh et al., Nature 418, 40 (2002).

TT 31.4 Thu 14:45 HSZ 301

Surface acoustic wave investigations of the metal-to-insulator transition of V_2O_3 thin films — •Claus Müller, Alexei A. Nateprov, Günter Obermeier, Matthias Klemm, Reinhard Tidecks, Achim Wixforth, and Siegfried Horn — Institut für Physik, Universität Augsburg, D-86159, Augsburg, Germany

A sensitive tool to study the lattice and electronic system of thin solid films are surface acoustic waves (SAW) generated on a piezoelectric substrate on which the material of interest is attached. By electron-beam evaporation a V_2O_3 film was deposited onto piezoelectric $LiNbO_3$. To investigate the metal-to-insulator (MI) transition surface acoustic wave studies were performed in a temperature range from 260K to 10K. The attenuation becomes maximal at the MI-transition and shows a hysteresis not only of electronic nature. The sound velocity change reveals a precursor of the MI-transition of V_2O_3 [1], which can also be detected in the attenuation using a self-retuning SAW delay line.

[1] C. Müller, A. A. Nateprov, G. Obermeier, M. Klemm, R. Tidecks, A. Wixforth, and S. Horn, J. Appl. Phys. **98**, 084111 (2005)

TT 31.5 Thu 15:00 HSZ 301

Evidence for dimer formation in XPS investigation of VO_2 — •T.C. Koethe[1], Jan Gegner[1], Z. Hu[1], F. Venturini[2], N.B. Brookes[2], W. Reichelt[3], and L.H. Tjeng[1] — [1]II. Physikalisches Institut der Universität zu Köln — [2]ESRF, Grenoble, France — [3]Institut für Anorganische Chemie, TU Dresden

VO_2 is a non-magnetic d^1-system that undergoes a metal-to-insulator transition (MIT) at 340K. Above this temperature VO_2 is metallic and has a rutile structure (R-phase). At low temperatures it is an insulator with a monoclinic structure (M_1-phase) in which V-V pairs are formed.

The long standing debate about this compound concerns the nature of the MIT. The issue is whether it can be regarded as a Peierls-transition with the character of a band insulator (one electron picture) or whether it should be viewed as a Mott-insulator (many-body-picture). Recently the scenario of an orbital assisted MIT has been proposed on the basis of the dramatic change of the orbital occupation across the MIT as observed by soft-X-ray absorption spectroscopy measurements.[1]

We present the results of our photoemission investigation of the MIT in VO_2 using high quality single crystals and 700eV photon energy. We observe a huge transfer of spectral weight across the MIT and a pronounced two peak structure in the R-phase, supporting recent LDA+DMFT cluster calculations.[2] Similar features are also observed in the insulating phase of the d^1-system Ti_2O_3. The origin of this double peak structure in the insulating phase can be related to the formation of dimers.

[1] M.W. Haverkort *et al.*, Phys. Rev. Lett. **95**, 196404 (2005)
[2] S. Biermann *et al.*, Phys. Rev. Lett. **94**, 026404 (2005)

TT 31.6 Thu 15:15 HSZ 301

Orbital fluctuations and Mott gap in $LaVO_3$ and YVO_3 — •E. Pavarini[1], M. Raychaudhury[2], and O.K. Andersen[2] — [1]IFF-Forschungzentrum Juelich, D-52425 Germany — [2]MPI-FKF, Heisenbergstrasse 1, D-70569 Stuttgart

The Mott insulators $LaVO_3$ and YVO_3 have attracted a lot of attention because of their anomalous magnetic and electronic properties, which are ascribed to the interplay bewteen orbital (t_{2g}) degrees of freedom, lattice and Coulomb repulsion. Here, by using the Nth-order Muffin Tin Orbital (NMTO)-based downfolding procedure, we construct a low energy Hubbard Hamiltonian for the partially filled t_{2g} bands; we than solve this Hamiltonian by means of LDA+DMFT, and obtain the full self-energy matrix in orbital space; we have already applied successfully this approacht to the series of $3d^1$ perovskites [1]. We will show that, in the case of $LaVO_3$ and YVO_3, orbital fluctuations are strong (more for $LaVO_3$ than for YVO_3) in the high temperature paramagnetic phase, and that they play an important role also in the low temperature magnetic phases. The interplay between filling, Coulomb repulsion, crystal field splitting and band widths is discussed, and their role in determining the size of the Mott gap in $LaVO_3$ and YVO_3 clarified.

[1] E. Pavarini, S. Biermann, A. Poteryaev, A.I. Lichtenstein, A. Georges, and OK Andersen, PRL **92** 176403 (2004).

TT 31.7 Thu 15:30 HSZ 301

Polarization- and temperature-dependent Ru-$L_{2,3}$ XAS study of Ca_2RuO_4 — •T. Burnus[1], Z. Hu[1], T. T. Tran[2], T. Mizokawa[2], H. H. Hsieh[3], L.-Y. Jang[4], S. Nakatsuji[5], Y. Maeno[5,6], M. Braden[1], K. S. Liang[4], and L. H. Tjeng[1] — [1]II. Phys. Inst., Univ. zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Dep. of Physics, Univ. of Tokyo, Bunkyo-ku, Tokyo 113, Japan — [3]Chung Cheng Inst. of Tech., National Defense Univ., Taoyuan 335, Taiwan — [4]Nat. Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30077, Taiwan — [5]Dep. of Physics, Kyoto Univ., Kyoto 606-8501, Japan — [6]Intern. Innov. Center, Kyoto Univ., Kyoto 606-8501, Japan

In the quasi-two-dimensional $Ca_{1-x}Sr_xRuO_4$, the strong correlations due to narrow electron bands and the active orbital degree of freedom yield a wide range of interesting properties. Ca_2RuO_4 has a transition at 350 K from a paramagnetic metal to a paramagnetic insulator and, cooling further down, it turns at 110 K into an antiferromagnetic insulator. We carried out polarization- and temperature-dependent X-ray absorption spectroscopy (XAS) at the Ru-$L_{2,3}$ edges in order to determine the occupation of the Ru 4*d* orbitals and their changes crossing the phase transitions; until now the occupation has been only obtained from O-*K* XAS, which contrary to the Ru-$L_{2,3}$ XAS only indirectly contains this information via the hybridization of the oxygen 2*p* with the ruthenium 4*d* orbitals. We observed the hysteretic change of the orbital occupation crossing the phase transitions. Furthermore, we confirmed the recently found additional phase transition around 260 K (Zegkkinglou *et al.* PRL, 2005).

TT 31.8 Thu 15:45 HSZ 301

New perspectives on charge ordering phenomena in complex transition-metal oxides — •Y. Su[1], H.F. Li[1], A. Nefedov[2], J. Persson[1], P. Meuffels[1], J. Grabis[2], H. Zabel[2], D. Wermeille[3], V. Kaiser[4], D. Schrupp[5], R. Claessen[5], V.A.M. Brabers[6], D. Prabhakaran[7], A.T. Boothroyd[7], P.D. Hatton[8], and Th. Brueckel[1] — [1]Institut für Festköperforschung, Forschungszentrum Juelich, D-52425 Juelich — [2]Inst. für Experimentalphysik IV, Ruhr-Universität Bochum — [3]MuCAT, Advanced Photon Source, Argonne National Laboratories — [4]Inst. für Kristallographie, RWTH — [5]Experimental Physik IV, Universität Wüzburg — [6]Dept. of Phys., Eindhoven University of Technology — [7]Dept. of Phys., Univ. of Oxford — [8]Dept. of Phys., Univ.of Durham

New insights on the nature of charge ordering in transition-metal oxides (TMO) have been gained via the latest resonant scattering experiments carried out in both soft (< 1 KeV) and hard (˜ 8 KeV) X-ray regimes on high-quality single crystals of lightly hole-doped La7/8Sr1/8MnO3 and mixed-valence Fe3O4. A giant resonance at the oxygen K absorption edge has been observed from the charge ordering superstructure reflections of both compounds, suggesting that the charge ordering is strongly associated with a spatial modulation of ligand-hole states near the Fermi surface. Comprehensive data obtained at the corresponding L3/L2 and K-edges also strongly supports this scenario. These investigations not only allow us to resolve the long-standing puzzles concerning the nature of the Verway transition, but also indicate that the localized ligand holes might be a key ingredient for many charge-transfer type TMO.

TT 31.9 Thu 16:00 HSZ 301

Bandwidth-controlled Mott transition in κ-phase BEDT-TTF salts — •Martin Dressel[1], N. Drichko[1], M. Dumm[1], D. Faltermeier[1], C. Meziere[2], and P. Batail[2] — [1]1. Phys. Inst., Univ. Stuttgart, Germany — [2]Lab. CIMI, CNRS-Univ. d'Angers, France

Infrared reflection measurements of the half-filled two-dimensional organic conductors κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br_xCl_{1-x}$ are performed as a function of temperature and Br-substitution ($x = 0\%$, 40%, 73%, 85%, and 90%) in order to study the metal-insulator transition. The mid-infrared band centered around 3400 cm^{-1} for $E \parallel c$ is assigned to localized charge transfer within the dimers which is barely visible along the *a* direction. As the charge becomes delocalized for increasing Br content and low temperatures, the band shifts to higher frequencies. In a similar way, intramolecular vibrations which are observed via electron-molecular vibration coupling change in frequency. As the temperature drops below 50 K an energy gap develop in the Cl-rich samples which increase for $T \to 0$. With increasing Br concentration spectral weight shifts into the gap region and eventually fills it up completely. As these samples ($x = 85\%$ and 90%) become metallic at low temperatures, a Drude-like component develops due to the coherent quasiparticles. We perform a detailed analysis of the spectral weight transfer which gives us insight into the influence of electronic correlations on the dynamical properties. The observed behavior of the Drude spectral weight at the critical value of U/t (which is reached for $x \approx 70\%$) agrees with the abrupt jump to a finite value predicted by theory. The series of alloys is a good model of a bandwidth-controlled Mott insulator.

— 15 min. break —

TT 31.10 Thu 16:30 HSZ 301

Signature of collective excitations close to the metal-to-insulator transition — •Götz Uhrig[1], Carsten Raas[1], and Michal Karski[2] — [1]FR 7.1, Geb. E2.6, Universität des Saarlandes, D-66123 Saarbrücken — [2]Insitut für Angewandte Physik, Universität Bonn, D-53115 Bonn

A high-resolution calculation of the dynamical mean-field equations for the half-filled Hubbard model reveals a clear signature of collective excitations close to the metal-to-insulator transition. This calculation has become possible by current advances in dynamical density-matrix renormalization. The effect of collective excitations is seen as sharp peaks at the inner edges of the Hubbard bands. These peaks evidence a strong interaction between charge and collective degrees of freedom. The corresponding susceptibilities display signatures of the involved collective modes.

TT 31.11 Thu 16:45 HSZ 301

Orbital-selective Mott transitions in Hubbard models with orbital-dependent hopping — •Nils Blümer, Carsten Knecht, Krunoslav Požgajčić, and Peter van Dongen — Institut für Physik, Johannes Gutenberg - Universität, 55099 Mainz

The anisotropic degenerate two-orbital Hubbard model is studied within dynamical mean-field theory at low temperatures. High-precision calculations on the basis of a refined quantum Monte Carlo (QMC) method reveal that two distinct orbital-selective Mott transitions occur for a bandwidth ratio of 2 even in the absence of spin-flip contributions to the Hund exchange. The second transition – not seen in earlier studies using QMC, iterative perturbation theory, and exact diagonalization – is clearly exposed in a low-frequency analysis of the self-energy and in local spectra. These published [1] results are complemented with recent studies using QMC and Potthoff's self-energy functional method.

[1] C. Knecht, N. Blümer, and P.G.J. van Dongen, Phys. Rev. B **72**, 081103(R) (2005).

TT 31.12 Thu 17:00 HSZ 301

Continuous-time quantum Monte Carlo Scheme for Multi-orbital Impurity Problems — •Evgeny Gorelov[1], Alexey Rubtsov[2], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg — [2]Department of Physics, Moscow State University, 119992 Moscow, Russia

A determinantal continuous-time quantum Monte Carlo (CTQMC) algorithm has been applied for the numerically exact calculation of the fermionic multiorbital impurity path-integral. The five-band model for realistic transition metal atoms with full Coulomb interaction vertex as Kondo impurities in a metal matrix is calculated. The metal-insulator phase transition for two and three anisotropic orbitals on the Bethe lattice with spin-flip interactions is considered. The obtained results are in good agreement with available previous studies. Application to a cobalt impurity in the copper matrix shows the formation of a many-body Abrikosov-Suhl-Kondo resonance near the Fermi level.

TT 31.13 Thu 17:15 HSZ 301

Spectral properties of correlated materials — •Jan M. Tomczak — Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France

Strong Coulomb interactions in solids can give rise to phenomena in the electronic excitation spectrum that lie beyond the one-particle picture, and are thus not accessible by density functional theory in the local density approximation (LDA), or any static treatment of the correlations (as in LDA+U). Among these are large transfers of spectral weight, the appearance of satellite structures and non-negligeable lifetime effects. By means of analytical continuation of Quantum Monte-Carlo data obtained within the framework of LDA + Dynamical Mean-Field Theory, we determine the real-frequency selfenergy for realistic materials. Therewith interesting quantities, such as k-resolved spectral functions, quasi-particle

bands and optical conductivities become accessible. We discuss technical aspects of the scheme, and, as an application, we make predictions for angle resolved photoemission spectra of vanadium dioxide.

TT 31.14 Thu 17:30 HSZ 301

Gapped and gapless phases of the Hubbard model with disorder — •Krzysztof Byczuk[1], Walter Hofstetter[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institut of Theoretical Physic A, RWTH Aachen, Templergraben 55, 52056 Aachen, Germany

The ground state phase diagram of correlated electrons with disorder is calculated within dynamical mean-field theory using the geometrically averaged ("typical") local density of states. The transitions between different gapped and gapless phases (paramagnetic, antiferromagnetic, Anderson localized) are described. In particular, the metal-insulator transition due to electronic correlations ("Mott-Hubbard transition") and disorder ("Anderson localization"), respectively, and the transition between a Slater and a Heisenberg antiferromagnet are discussed. The staggered magnetization is calculated as a function of disorder strength and interaction.

K. Byczuk, W. Hofstetter, and D. Vollhardt, Phys. Rev. Lett. 94, 056404 (2005); Physica B 359-361, 651 (2005).

TT 31.15 Thu 17:45 HSZ 301

Stochastic Green's function approach to disordered systems — •Andreas Alvermann and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, 17487 Greifswald, Germany

We adopt a stochastic approach based on distributions of Green's functions to study the electronic structure of disordered systems. Exemplarily, we address Anderson localisation as well as cluster effects in binary alloys. Combining this stochastic Green's function approach with dynamical mean field theory, we investigate the competition between polaron formation and Anderson localisation in a generic model for a disordered electron-phonon system.

TT 31.16 Thu 18:00 HSZ 301

Effective model for $E \otimes \beta$-coupling and electron-electron interaction — •Daniela Schneider, Klaus Ziegler, and Karl-Heinz Höck — Institut für Physik, Universität Augsburg, 86135 Augsburg

We investigate the effect and interplay of orbital and spin degrees of freedom. The model takes electron-electron interaction and electron-phonon coupling of the $E \otimes \beta$-type into account. The hopping is considered as orbital conserving. We derive an effective spin-orbital Hamiltonian at quarter filling through projection on singly occupied sites, treating the phonons quantummechanically, and discuss the symmetry of the initial and the effective model. Furthermore we identify the similarities and differences to the purely electronic and the adiabatic effective Hamiltonian. The anisotropy in the orbital part reflects the difference of spin and orbital exchange. The groundstate properties are studied for small clusters and the influence of the electron-phonon interaction and the spin and orbital occupancy are investigated. For dimers we compare the results obtained by exact diagonalisation with those achieved with the effective Hamiltonian.

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TT 31.17 Thu 18:15 HSZ 301

Transport properties of polaronic systems at finite temperature — •Alexander Weisse[1], Andreas Alvermann[1], Gerald Schubert[1], Gerhard Wellein[2], and Holger Fehske[1] — [1]Theoretische Physik II, Universität Greifswald, 17487 Greifswald — [2]RRZ Erlangen, Universität Erlangen, 91058 Erlangen

We review recent developments of Chebyshev expansion based algorithms for the calculation of dynamical correlation functions and apply these techniques to the one-dimensional Holstein model. Focussing on the case of finite temperatures, we present exact numerical results for the optical response in this prototypical model for electron-lattice interaction. In addition, we analyze deviations from the standard small polaron theory in the intermediate coupling regime and discuss non-adiabaticity effects in detail. [Phys. Rev. B 72, 104304 (2005)]