TT 43: Correlated Electrons: Metal-Insulator Transition 2

Time: Wednesday 15:00–16:30 Location: H19

TT 43.1 Wed 15:00 H19

Charge self-consistent DFT+DMFT approach to strong correlation effects in transition-metal oxides — •Frank Lechermann[1], Daniel Grieger[1], Oleg. E. Peil[2], and Christoph Piefke[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Department of Condensed Matter Physics, University of Geneva

One of the most suited class of materials to study the physics of strongly correlated electron systems in a realistic scenario is provided by a group of transition-metal oxides. The specific chemistry of these compounds allows for rather localized states in the solid state, giving rise to a variety of intricate phenomena. Large-gap insulators, systems close to a metal-insulator transition as well as metals with an enormously high conductivity all belong to these materials. It will be shown that the newly developed charge self-consistent combination of density functional theory (DFT) and dynamical mean-field theory (DMFT) based on the projected-local-orbital interface between a mixed-basis pseudopotential method and the continuous-time quantum Monte Carlo impurity solution to DMFT [1], is capable of addressing the vast characteristics among correlated transition-metal oxides. For instance, the metal-insulator transition in V_2O_3 will be discussed.

[1] D. Grieger, C. Piefke, O. E. Peil and F. Lechermann, PRB **86**, 155121 (2012)

TT 43.2 Wed 15:15 H19

Orbital and spatial correlations in $LiVS_2$ from a two-particle perspective — •Lewin Boehnke and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

The compound $LiVS_2$ shows a transition from a paramagnetic metal to a trimerized valence bond solid insulator phase [1] at 310K. Such a behaviour is already known from its neighbouring compound $LiVO_2$. In contrast to previous studies that concentrated on the symmetry-broken insulating phase [2], our attention is on the emergence of this low-temperature phase from the high-temperature phase. We employ the formalism outlined in [3] to calculate lattice spin- and charge-susceptibilities for this system on top of density functional theory + dynamical mean-field theory (DFT+DMFT) calculations for a detailed investigation of non-local two-particle correlations in view of the orbital ordering and trimerization effects that are observed.

[1] N. Katayama, *et al.*, PRL **103**, 146405 (2009)
[2] H. Pen, *et al.*, PRL **78**, 1323 (1997)
[3] L. Boehnke, *et al.*, PRB **84**, 075145 (2011)

TT 43.3 Wed 15:30 H19

Correlation effects and spin-orbit interaction in $Sr_3Ru_2O_7$: LDA+DMFT study — •Evgeny Gorelov, Guoren Zhang, and Eva Pavarini — IAS-3, Forschungszentrum Jülich, 52425 Jülich

The layered ruthenates of the Ruddlesden-Popper family $Sr_{n+1}Ru_nO_{3n+1}$ are interesting examples of strongly correlated transition metal compounds. Due to competing kinetic and Coulomb energies, that are of the same order for Ru 4*d* electrons, these compounds have very rich phase diagram, including Mott-insulator, ferro- and meta-magnetic phases. Among layered ruthenates the bilayered compound $Sr_3Ru_2O_7$ is particularly interesting. It is known to be a paramagnetic metal close to ferro-magnetism and exhibits a metamagnetic behavior in external magnetic field. By using the LDA+DMFT (local-density approximation + dynamical mean-field theory) approach, we study magnetic properties and electron mass renormalization due to correlation effects. In our LDA+DMFT scheme we use maximally-localized Wannier orbitals obtained from Linearized Augmented Plane Wave (LAPW) calculations to build a low-energy Hubbard model for the Ru *d* bands; we use the weak-coupling CT-quantum Monte Carlo method to solve the quantum impurity problem. We 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.

[1] E. Gorelov, G. Zhang, and E. Pavarini, Correlation effects and spin-orbit coupling in $Sr_{n+1}Ru_nO_{3n+1}$ compounds (in preparation)

TT 43.4 Wed 15:45 H19

LDA+DMFT calculations of the Knight shift and relaxation rate in $VOMoO_4$ — •Amin Kiani and Eva Pavarini — Institute for Advanced Simulation and JARA, Forschungszentrum Jülich, 52425 Jülich, Germany

By using the LDA+DMFT approach and the local vertex approximation, we calculate the magnetic linear response function of strongly correlated transition-metal oxides. From the susceptibility we obtain Knight shift and relaxation rate. We present results for the frustrated system $VOMoO_4$. In particular we investigate how the Knight shift and the relaxation time behave in different temperature and correlation regimes.

TT 43.5 Wed 16:00 H19

DFT + DMFT calculations for epitaxially strained $LaTiO_3$ — •Krzysztof Dymkowski and Claude Ederer — Materials Theory, ETH Zurich, Switzerland

Even though bulk $LaTiO_3$ is a Mott insulator [1], metallic properties have been reported for thin films of $LaTiO_3$ grown on $SrTiO_3$ [2]. Such metallicity, can be due to a number of factors such as: electronic reconstruction at the interface, defects, or substrate-induced structural deformations. In order to identify the origin of the observed metallicity, we perform density functional theory plus dynamical mean field theory (DFT + DMFT) calculations for epitaxially strained $LaTiO_3$. First, we use standard DFT to accurately relax the structure under the epitaxial constraint, and we monitor hopping amplitudes and crystal-field splitting as a function of strain. Then, we calculate the electronic properties for the strained structures using DMFT. Based on our results we address the question whether the strain-induced structural modifications of $LaTiO_3$ are enough to change this insulator into a metal.

[1] E. Pavarini et al., Phys. Rev. Lett. 92, 176403 (2004)
[2] F. J. Wong et al., Phys. Rev. B 81, 161101 (2010); C. He et al., Phys. Rev. B 86, 081401 (2012)

TT 43.6 Wed 16:15 H19

Magnetic susceptibility of the orbital-selective Mott phase — •Markus Greger, Michael Sekania, Marcus Kollar, and Dieter Vollhardt — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg

We analyze the low-energy physics of multi-orbital Hubbard models in the orbital-selective Mott phase within Dynamical Mean-Field Theory. Our main focus lies on the calculation of dynamical two-particle quantities, e.g., susceptibilities. They are of particular interest in these systems since the coupling between the orbitals is not due to a hybridization, but is caused by two-particle processes originating from the interaction, i.e., the Hund's rule coupling J and the inter-orbital repulsion U_1. Employing the Numerical Renormalization Group as an impurity solver we obtain diverging spin-susceptibilities $\chi^{sp}_{i,j}(\omega)$ at $\omega = 0$; here i, j are orbital indices. This corresponds to a divergent density of states for magnetic excitations, indicative of an instability of the phase. An explanation based on a Kondo-type Hamiltonian is given. These results also provide a better characterization of the known non-Fermi liquid properties of the phase.