

TT 86: Correlated Electrons: Other Materials

Time: Thursday 9:30–12:45

Location: BEY 81

TT 86.1 Thu 9:30 BEY 81

Metal-insulator transition in LiVS_2 through correlation-induced orbital-spin ordering — LEWIN BOEHNKE, ALEXANDER I. LICHTENSTEIN, and ●FRANK LECHERMANN — I. Institute for Theoretical Physics, University of Hamburg

The investigation of nature's various mechanisms to localize electrons within a material that undergoes a metal-insulator transition (MIT) is a salient research endeavour in condensed matter physics. Prominent localization driving forces in the chemically ordered states are either dominant exchange processes, giving rise to a Slater insulator, or strong correlations, leading to an insulator of Mott type. However in complex compounds with manifest multi-orbital character and apparent geometrical frustration the many-body physics underlying the competition between metallic and insulating state may even be more intricate. Here the advanced combination of density functional theory with dynamical mean-field theory including multi-orbital vertex contributions to determine (dynamic) lattice susceptibilities in the strong correlation regime is used to study the nebulous MIT in quasi-two-dimensional LiVS_2 . Entangled orbital-spin ordering tendencies originating in the high-temperature metallic phase are revealed. Those lead to a transition into a challenging insulating phase close to room temperature.

TT 86.2 Thu 9:45 BEY 81

The insulating phases of Vanadium Sesquioxide (V_2O_3) — ●DANIEL GRIEGER¹, FRANK LECHERMANN², and MICHELE FABRIZIO¹ — ¹SISSA - Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy — ²I. Institut für Theoretische Physik, Universität Hamburg, Germany

Vanadium Sesquioxide (V_2O_3) has attracted large attention mainly because of its prototypical Mott insulating behaviour with negative (chemical) pressure/Chromium doping. Besides trying to shed some light on the actual difference between doping and pressure in view of electronic correlations modelled by the charge self-consistent LDA+DMFT approach, this contribution is primarily aimed at the low-temperature ($T < 140\text{K}$) antiferromagnetic insulating phase, which has not been properly understood for the last 40 years. It shows a peculiar magnetic ordering involving ferromagnetic out-of-plane bonds and two antiferromagnetic/one ferromagnetic in-plane bond per Vanadium atom, at the additional energetic cost of a monoclinic structural distortion. Arguments about why this complicated structure turns out to be stable are given from a combination of traditional electronic structure formalisms and DFT+-like approaches.

TT 86.3 Thu 10:00 BEY 81

May the character of the metal-insulator transition of disordered materials be determined by how one looks at it? — ●ARNULF MÖBIUS — Institute for Theoretical Solid State Physics, IFW Dresden

In a recent experiment, Siegrist et al. studied the metal-insulator transition (MIT) of phase-change materials [1]. They conclude that these substances exhibit a finite minimum metallic conductivity. The striking contrast to reports on other disordered substances motivates the present study of the influence of the MIT criterion used on the character of the MIT obtained [2]. First, we discuss inherent biases of various approaches to locating the MIT. Second, reanalyzing GeSb_2Te_4 data from [1], we show that this solid strongly resembles other disordered materials: The data may also be interpreted in terms of a continuous MIT. Checking the justification of these fits, however, uncovers data inconsistencies preventing an unambiguous interpretation. Third, comparing with previous experiments on crystalline Si:As, Si:P, Si:B, Ge:Ga, disordered Gd, and nano-granular Pt-C, we show that such an inconclusive behavior occurs frequently: The logarithmic temperature derivative of the conductivity highlights serious inconsistencies in the original interpretations in terms of a continuous MIT. Thus, the question for the character of the MIT of these materials has to be considered as yet open. The primary challenge lies in improving the measurement precision rather than extending the temperature range.

[1] T. Siegrist et al., Nature Materials 10 (2011) 202.

[2] A. Möbius, arxiv.org/abs/1308.1538.

TT 86.4 Thu 10:15 BEY 81

Non-magnetic ground state of PuO_2 — ●JINDRICH KOLORENC¹,

ALEXANDER B. SHICK¹, LADISLAV HAVELA², THOMAS GOUDER³, and ROBERTO CACIUFFO³ — ¹Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — ²Charles University, Prague, Czech Republic — ³European Commission, Joint Research Centre, Institute for Transuranium Elements, Karlsruhe, Germany

The correlated band theory implemented as a combination of the local density approximation with the exact diagonalization of the Anderson impurity model is applied to PuO_2 . We obtain an insulating electronic structure consistent with the experimental photoemission spectra. The calculations yield the band gap of 1.8 eV and a non-magnetic singlet ground state that is characterized by a non-integer filling of the plutonium f shell ($n_f \approx 4.5$). Due to sizeable hybridization of the f shell with the p states of oxygen, the ground state is more complex than the four-electron Russell-Saunders 5I_4 manifold split by the crystal field. The inclusion of hybridization improves the agreement between the theory and experiment for the magnetic susceptibility.

TT 86.5 Thu 10:30 BEY 81

The origin of orbital and magnetic order in K_2CuF_4 — ●GUOREN ZHANG¹, ERIK KOCH², and EVA PAVARINI¹ — ¹Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — ²German Research School for Simulation Sciences, 52425 Jülich, Germany

In this work, we investigate the origin of magnetic and orbital order in K_2CuF_4 . We first construct Wannier functions from the Bloch states obtained by local-density approximation calculations with the full-potential linearized augmented plane-wave method. Then, by perturbative theory, we calculate magnetic couplings which are in good agreement with experimental results both for the ambient and high pressure structures. To investigate the origin of orbital order, we perform calculations with local-density approximation+dynamical mean-field theory method. We discuss the roles of crystal-field[1], superexchange and the charge-transfer effects[2] on the orbital ordering.

[1] K. I. Kugel and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)].[2] M.V. Mostovoy and D. I. Khomskii, Phys. Rev. Lett. **92**, 167201 (2004).

TT 86.6 Thu 10:45 BEY 81

On the orbital-ordering transition in KCuF_3 — ●HUNTER SIMS¹, EVA PAVARINI², and ERIK KOCH¹ — ¹German Research School for Simulation Sciences, 52428 Jülich, Germany — ²Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

The Mott insulating perovskite KCuF_3 is considered the paradigmatic system with long-ranged orbital order and a cooperative Jahn-Teller distortion of the F-octahedra. This broken symmetry state is usually understood as the result of the destabilization of the symmetric structure due to crystal-field splitting (Jahn-Teller effect) or to superexchange between the orbitals (Kugel-Khomskii mechanism), which leads to a gain in energy with increasing distortion. This is counteracted by the quadratic deformation energy of the lattice. In this picture it is expected that, as a consequence of the lattice entropy, the distortions will be gradually reduced with increasing temperature until they finally vanish at the ordering temperature T_c . Such a transition is, however, not found experimentally. We explain why.

15 min. break.

TT 86.7 Thu 11:15 BEY 81

Fermi surface of $\text{Sr}_{n+1}\text{Ru}_n\text{O}_{3n-1}$ ruthenates: LDA+DMFT study — ●EVGENY GORELOV, GUOREN ZHANG, and EVA PAVARINI — IAS, Forschungszentrum Jülich, 52425 Jülich

The layered ruthenates of the Ruddlesden-Popper family $\text{Sr}_{n+1}\text{Ru}_n\text{O}_{3n+1}$ are interesting examples of strongly correlated transition metal compounds. Because kinetic and Coulomb energy are of the same order for Ru 4d electrons, these compounds have a very rich phase diagram. Furthermore, the spin-orbit coupling (SOC) is comparable with crystal-field splitting of t_{2g} levels and it is thus crucial for the description of the Fermi surface.

In the present work we focus on three compounds of the $\text{Sr}_{n+1}\text{Ru}_n\text{O}_{3n+1}$ family: single-layered Sr_2RuO_4 , double layered $\text{Sr}_3\text{Ru}_2\text{O}_7$, and triple-layered $\text{Sr}_4\text{Ru}_3\text{O}_{10}$. We study the shape of

the Fermi surface and the electron mass renormalization in the presence of correlation effects and SOC. In our LDA+DMFT (local-density approximation + dynamical mean-field theory) scheme we use maximally-localized Wannier orbitals obtained from Linearized Augmented Plane Wave (LAPW) ab-initio calculations to build a low-energy Hubbard model for the Ru $4d$ bands; we use the weak-coupling 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 spin-orbital space. For $\text{Sr}_4\text{Ru}_3\text{O}_{10}$ we use the cluster DMFT scheme to account for the inequivalent Ru atoms.

TT 86.8 Thu 11:30 BEY 81

Metal-insulator and magnetic transitions of Ca_2RuO_4 observed by hard x-ray photoemission spectroscopy — •YUKI UTSUMI¹, STEFANO AGRESTINI¹, ZHIWEI HU¹, KYUNG-TAE KO¹, KU-DING TSUEI², YEN-FA LIAO², YU-HAN WU², KOMAREK C. ALEXANDER¹, and LIU HAO TJENG¹ — ¹Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — ²National Synchrotron Radiation Research Center, Hsinchu, Taiwan

Layered perovskite Ca_2RuO_4 has been attracting a great interest as much as the spin triplet superconductor Sr_2RuO_4 because of its rich properties. Isovalent Ca substitution for Sr changes the system from superconductor to Mott insulator. Ca_2RuO_4 is an antiferromagnetic insulator below $T_N=110$ K and exhibits a metal-insulator transition (MIT) at ~ 357 K accompanied by a crystal structure distortion. The MIT temperature continuously decreases with increase in Sr content. For the case of $\text{Ca}_{1.91}\text{Sr}_{0.09}\text{RuO}_4$, the MIT temperature becomes almost equal to T_N . Despite a large number of experimental and theoretical studies, the mechanism of the MIT in Ca_2RuO_4 is still hotly debated. Here we report a hard x-ray photoemission spectroscopy (HAXPES) study of the electronic structure of this layered system as a function of temperature. The valence-band spectrum of Ca_2RuO_4 shows dramatic changes across the MIT. The valence band spectrum of $\text{Ca}_{1.91}\text{Sr}_{0.09}\text{RuO}_4$ displays similar temperature evolution across the MIT. These HAXPES results indicate not only a rearrangement in t_{2g} orbital occupation but also the importance of electronic correlations for the MIT.

TT 86.9 Thu 11:45 BEY 81

HAXPES study of the spectral weight distribution of d^1 Mott insulators LaTiO_3 — •JONAS WEINEN¹, STEFANO AGRESTINI¹, ALEXANDER C. KOMAREK¹, ZHIWEI HU¹, THOMAS KOETHE², MAURITS W. HAVERKORT¹, YEN-FA LIAO³, KU-DING TSUEI³, and LIU H. TJENG¹ — ¹Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — ²II. Physikalisches Institut der Universität zu Köln — ³National Synchrotron Radiation Research Centre, Hsinchu, Taiwan

Using hard x-ray photoelectron spectroscopy (HAXPES) we have obtained bulk-sensitive valence band spectra of the d^1 Mott insulators LaTiO_3 and YTiO_3 . The experiment was performed in the s polarization, thus suppressing the s orbitals spectral weight which hide the d orbitals when using the more common p polarization.

We observed appreciable differences between the spectra of the two compounds, reflecting the difference in the one-electron band width. We also found that the Ti $3d$ spectra of both materials are much broader than the occupied $3d$ bands calculated by band theories. The mean-field inclusion of the Hubbard U explains the band gap but produces even narrower bands, indicating the complete breakdown of standard meanfield theories in describing excitation spectra. We associate the observed spectra with the propagation of a hole in a system with surprisingly well suppressed charge fluctuations thereby showing characteristics of a t - J model.

TT 86.10 Thu 12:00 BEY 81

Topological superconducting phases in the doped Kitaev-Heisenberg model — •DANIEL SCHERER¹, MICHAEL SCHERER², GINIYAT KHALIULLIN³, CARSTEN HONERKAMP^{4,5}, and BERND ROSENOW¹ — ¹Institute for Theoretical Physics, University of Leipzig, D-04103 Leipzig, Germany — ²Institute for Theoretical Physics, University of Heidelberg, D-69120 Heidelberg, Germany — ³Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — ⁴Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52056 Aachen, Germany — ⁵JARA Fundamentals of Future Information Technologies

The Kitaev-Heisenberg model can describe the magnetic ground-state of the spin-orbit Mott insulator Na_2IrO_3 . Here, we present our analysis of the quantum many-body instabilities found in the doped system within the framework of a t - J model. We determine ordering tendencies by the functional renormalization group (fRG) method for correlated fermionic systems in an unbiased way. To this end, we derived fRG flow-equations and Ward identities adapted to the lack of full spin-rotational invariance in the fermionic interactions caused by the highly anisotropic and frustrated Kitaev exchange. The solution of the flow equations suggests a rich phase diagram emerging upon doping charge carriers into the ground-state manifold (quantum spin liquids, magnetically ordered phases) of the Kitaev-Heisenberg Hamiltonian. We confirm superconducting triplet p -wave instabilities driven by ferromagnetic exchange. These p -wave phases turn topological upon increasing doping-level and support Majorana edge-modes.

TT 86.11 Thu 12:15 BEY 81

Investigation of the Verwey transition in Fe_3O_4 thin films — •XIONGHUA LIU, DIANA RATA, CHUN FU CHANG, ALEXANDER KOMAREK, and LIU HAO TJENG — Max Planck Institute for Chemical Physics of Solids, Dresden

Magnetite Fe_3O_4 is one of the most investigated materials from the class of correlated transition metal oxides. It shows a first-order anomaly in the temperature dependence of the electrical conductivity at $T_V = 125$ K, the famous Verwey transition. However, thin films of Fe_3O_4 show always a lower T_V compared to the bulk material. In order to find out the reason for the decreased T_V in magnetite thin films we have performed a systematic investigation of the transport properties in dependence of the oxygen pressure and thickness. Having found the optimum conditions for the growth of fully stoichiometric Fe_3O_4 thin films, we vary the substrate and study the influence of the microstructure on the Verwey transition. We are now able to obtain Fe_3O_4 thin films with T_V higher than the bulk value.

TT 86.12 Thu 12:30 BEY 81

Hund's and lattice coupling as origin of the insulating state in BaCrO_3 — •MARKUS AICHHORN¹, GIANLUCA GIOVANNETTI², and MASSIMO CAPONE² — ¹Institute of Theoretical and Computational Physics, TU Graz, Austria — ²SISSA, Trieste, Italy

Strong correlations play an important role for the physical properties in many oxide materials. Since most of these materials are multi-band systems, the Hund's rule coupling turns out to be a key player for the occurrence of sizeable electron correlations. Recently, insulating behavior has been found in layered BaCrO_3 , which cannot be explained by density-functional theory calculations. Here, we will show that Hund's coupling, orbital, and lattice degrees of freedom cooperate in turning this system with 2 electrons in 3 bands to an insulator. The orbital degrees of freedom are also strongly coupled to spins leading to a magnetic transition with large magnetic moments. We argue that the so-called Hund's correlated metals are very unstable towards perturbations such as Jahn-Teller distortions and orbital ordering.