TT 38: Correlated Electrons: Metal-Insulator Transition 1

Time: Wednesday 9:30–13:15 Location: H20

TT 38.1 Wed 9:30 H20

Verwey Transition in epitaxial Fe_3O_4 thin films studied by Raman spectroscopy — •Mehrdad Baghaie Yazdi[1], Kwang-Yong Choi[2], Dirk Wulferding[3], Peter Lemmens[3], and Lambert Alff[1] — [1]TU Darmstadt, Materialwissenschaft — [2]Chung-Ang University, Department of Physics, Seoul, Korea — [3]TU Braunschweig, Institut für Festköperphysik

Magnetite has served as the model material for metal insulator transitions for more than seven decades. However, the origin and nature of the Verwey transition remains debated to this day. Recent disputes over the interpretation of measurement data [1,2] have reignited the question over the fundamental driving force behind the Verwey transition. Currently two major models try to explain the origin of this phenomenon, namely one that postulates that the transition is structurally driven [3] while the other sees the ordering of the t_{2g} orbitals of the Fe^{2+} ions at the octahedral sites as the main cause for both charge localization and structural transformation. Using epitaxial thin films of magnetite grown on Al_2O_3 and MgO which exhibit different Verwey transition temperatures, 128 K and 119 K respectively, we have investigated the evolution of ordering peaks in Raman spectroscopy. These peaks have been correlated to the global magnetic and electric properties of the films measured by SQUID and four-point electrical transport measurements.

[1] A. Tanaka *et al.*, Phys. Rev. Lett. **108**, 227203 (2012).
[2] S. B. Wilkins *et al.*, Phys. Rev. B **79**, 201102(R) (2009).
[3] G. Kh. Rozenberg *et al.*, Phys. Rev. Lett. **96** 045705 (2006).

TT 38.2 Wed 9:45 H20

Strongly Correlated Material under Voltage: The Electrical Breakdown in V_2O_3 at the Insulator to Metal Transition — •Stefan Guénon[1], Sebastian Scharinger[2], Siming Wang[1], Juan Gabriel Ramírez[1], Dieter Koelle[2], Reinhold Kleiner[2], and Ivan K. Schuller[1] — [1]Department of Physics and Center for Advanced Nanoscience, University of California San Diego — [2]Physikalisches Institut and Center for Collective Quantum Phenomena and their Applications in LISA+, Universität Tübingen

We have investigated the electrical properties of a V_2O_3 thin film micro bridge. Discontinuous jumps to lower voltages in the current voltage characteristic (IV) followed by an approximately constant voltage progression for high currents indicate an electrical breakdown of the device. In addition, the IV curves show hysteresis and a training effect, i.e. the subsequent IV loops are different from the first IV loop after thermal cycling. Low temperature scanning electron microscopy (LTSEM) reveals that the electrical breakdown over the whole device is caused by the formation of electro-thermal domains (ETDs), i.e. the current and temperature redistribution. On the contrary, at the nanoscale, the electrical breakdown causes the insulator to metal transition of individual domains. In a numerical model we considered these domains as a network of resistors and we were able to reproduce the electro-thermal breakdown as well as the hysteresis and the training effect in the IVs.

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TT 38.3 Wed 10:00 H20

Nanodomain formation and electronic transport near the 1st-order Mott-Hubbard transition — Qinyong Liu and •Johann Kroha — Physikalisches Institut, Universität Bonn

In the vicinity of the 1st-order metal-insulator transition (MIT) in Mott-Hubbard systems metallic and insulating phases coexist. Since the MIT occurs not only at temperature $T = 0$, but persists to finite T, in the coexistence region the thermodynamically stable state consists of thermal excitations of insulating nanodomains within the metal and vice versa. The existence of such nanodomains has been demonstrated experimentally in VO_2. We calculate the size distribution of nanodomains as a function of T and Hubbard repulsion U. To that end, the electronic spectra and the free energy per site are determined in metallic and in insulating regions as well as across a metal-insulator domain wall, using the generalization of dynamical mean field theory (DMFT) for inhomogeneous systems, with the non-crossing approximation (NCA) as impurity solver. The domain-size distribution is then obtained from the resulting free energy difference, including volume and domain wall energies. It exhibits non-trivial, non-monotonic behavior. The 1st-order MIT of Mott-Hubbard systems may, hence, be viewed as a percolation problem with self-generated domain disorder. We calculate the electric resistivity $\rho(T)$ by mapping this problem of random nanodomains onto a random resistor network. Within the phase coexistence region, $\rho(T)$ exhibits anomalous linear T depenence.

TT 38.4 Wed 10:15 H20

Phase transitions induced by the cooperative Jahn-Teller effect: A multi-scale study of $KCuF_3$ — •Joaquin Miranda Mena[1], Erik Koch[1], and Eva Pavarini[2] — [1]German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University — [2]Institute for Advanced Simulation and JARA, Forschungszentrum Jülich

We study the transition temperature for the structural and the orbital ordering in $KCuF_3$. We first obtain temperature dependent dynamical matrices (TDM) of the crystalline phase by computing the energy displacements of fluorines with density functional theory (DFT) within the LSDA+U framework. Because of the Coulomb interactions, the TDM tend to be quite long ranged. To minimize the required amount of DFT calculations, we subtract the long rang Coulomb (LRC) interaction to obtain short ranged TDM that can be transformed to the disorder systems. The transition temperature is found through Monte Carlo simulations. Here the fluorine positions are sampled using the short-ranged TDM adding back the LRC by an Ewald summation; as a result disorder states can be computed fast and efficiently regardless of the size of system.

TT 38.5 Wed 10:30 H20

Electronic structure of $Nb_{0.75}O_{0.75}$ — •Anna Efimenko[1,2], Nils Hollmann[1], Katharina Höfer[1], Jonas Weinen[1], Alexander C. Komarek[1], Zhiwei Hu[1], A.Agung Nugroho[3], Hui-Huang Hsieh[4], Hong-Ji Lin[4], Chien-Te Chen[4], Aurora Diana Rata[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]II.Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Institut Teknologi Bandung, Jl. Ganesa 10 Bandung, 40132, Indonesia — [4]National Synchrotron Radiation Research Center (NSRRC), 101 Hsin-Ann Road, 30077 Hsinchu, Taiwan

We report on our angle-resolved photoemission (ARPES) study of $Nb_{0.75}O_{0.75}$ single crystals. NbO crystallizes in a rocksalt structure with 25% of ordered vacancies on both Nb - and O - sublattices. We compare our experimental data with the electronic structure calculated by density functional theory. Experimentally obtained bands are assigned to bulk and plausible surface electronic states. The effect of the so called "ordered vacancies" formation on the electronic structure in this compound is discussed. Our results demonstrate the shortcomings of the ionic model for $Nb_{0.75}O_{0.75}$ and the importance of metal-metal bonds for the structural stability. We provide insight into the bonding of Nb and O by constructing the topology of the orbitals from projected Wannier functions.

TT 38.6 Wed 10:45 H20

Importance of exchange anisotropy and superexchange for the spin-state transitions in $RCoO_3$ (R = rare earth) cobaltates — •Guoren Zhang[1], Evgeny Gorelov[1], Erik Koch[2,3], and Eva Pavarini[1,3] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]German Research School for Simulation Sciences, 52425 Jülich, Germany — [3]JARA High-Performance Computing

In this work [1], we identify all relevant parameters which shift the energy balance between spin states in rare-earth cobaltates, and determine their trends. We find that the e_g-t_{2g} crystal-field splitting increases by $\sim$ 250 meV when increasing pressure to 8 GPa, by about 150 meV when cooling from 1000 K to 5 K and by less than 100 meV when La is substituted with another rare earth. Hund's rule coupling is about the same in systems with very different spin-state transition temperature. In addition, the Coulomb-exchange anisotropy and the super-exchange energy-gain play a crucial role. In the $LnCoO_3$ series (Ln=Y or R), super-exchange progressively stabilizes a low-spin ground state as the Ln^{3+} ionic radius decreases. We use a simple model to describe spin-state transitions and show that, at low temperature,

the formation of isolated high-spin/low-spin pairs is favored, while in the high-temperature phase, the most likely homogeneous state is high-spin, rather than intermediate spin. An *orbital-selective* Mott state could be a fingerprint of such a state.

[1] G. Zhang, E. Gorelov, E. Koch and E. Pavarini, Phy. Rev. B **86** 184413 (2012)

TT 38.7 Wed 11:00 H20

Dielectric breakdown of Mott insulators – doublon production and doublon heating — •Martin Eckstein[1] and Philipp Werner[2] — [1]Max Planck Research Department for Structural Dynamics, University of Hamburg, CFEL — [2]University of Fribourg, Switzerland

Using nonequilibrium dynamical mean-field theory, we study the response of a Mott insulator to strong dc electric fields. Previously, the resulting dielectric breakdown of the insulating state has been studied for isolated bulk systems [1]. Remarkably, in this case a quasi-steady current is observed, although the energy of the system is constantly increasing. In this talk, we show that the current in this nonequilibrium quasi-steady state is related to a field-induced doublon-hole creation mechanism [2]. The induced carriers acquire an infinite-temperature distribution, and hence they do not contribute to the current after the initial pair-creation process. This observation allows to obtain a consistent understanding for the effects of high temperature and dissipation in those systems, which is essential for an understanding of bias-induced metal-insulator transitions in correlated systems.

[1] M. Eckstein, T. Oka, and Ph. Werner, Phys. Rev. Lett. 105, 146404 (2010)
[2] M. Eckstein, and Ph. Werner, arXiv:1211.2698.

15 min. break

TT 38.8 Wed 11:30 H20

Dimensional-crossover-driven Mott transition in the frustrated Hubbard model — •Marcin Raczkowski and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg

We study the Mott transition in a frustrated Hubbard model with next-nearest neighbor hopping at half-filling [1]. The interplay between interaction, dimensionality and geometric frustration closes the one-dimensional Mott gap and gives rise to a metallic phase with Fermi surface pockets. We argue that they emerge as a consequence of remnant one-dimensional Umklapp scattering at the momenta with vanishing interchain hopping matrix elements. Such a mechanism can also account for the pockets observed in the *spinless* model. In this pseudogap phase, enhanced d-wave pairing correlations are driven by antiferromagnetic fluctuations. Within the adopted cluster dynamical mean-field theory on the 8×2 cluster and down to our lowest temperatures the transition from one to two dimensions is continuous.

[1] M. Raczkowski and F. F. Assaad, Phys. Rev. Lett. **109**, 126404 (2012)

TT 38.9 Wed 11:45 H20

Effective singlet dynamics in Mott phases of two-dimensional Hubbard models — •Dominik Ixert and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

The Hubbard model is one of the paradigm models for the description of strongly correlated electron systems. In this work we focus on the intermediate-coupling regime inside the Mott insulating phase of single-band Hubbard models at zero temperature and at half filling. Recently, several works found indications for exotic spin-liquid phases close to the metal-insulator transition. While the situation on frustrated lattices like the triangular lattice concerning the existence of such interesting intermediate phases seems to be rather settled, the situation on unfrustrated lattices like the honeycomb lattice or the π-flux square lattice is currently under debate. In all these cases the Mott phase displays a long-ranged ordered antiferromagnet at strong couplings. Here our main focus is a class of two-dimensional systems for which the translational symmetry of the underlying square lattice is broken explicitly and the systems therefore realize a valence bond crystal at strong coupling. Consequently, one expects that the low-energy physics of the full Mott phase is contained in the singlet sector. For such systems we derive effective low-energy spin models using graph-based continuous unitary transformations (gCUTs). The effective spin models are then analyzed in the singlet sector by embedding the graphs within the dimer covering space on larger clusters to describe the singlet dynamics of the hubbard model.

TT 38.10 Wed 12:00 H20

Dual Fermions + Disorder — •Patrick Haase[1], Hanna Terletska[2], Shuxiang Yang[2], Thomas Pruschke[1], and Mark Jarrell[2] — [1]Georg-August Universität Göttingen — [2]Louisiana State University

We introduce an extension of the Dual Fermion formalism that allows to tread disordered interacting systems. To derive the formalism, the Replica trick is used. We will show data that compares the method to results obtained within the coherent potential approximation and the dynamical cluster approximation.

TT 38.11 Wed 12:15 H20

Numerical solution of the t-J model with random coupling in infinite dimensions — •Junya Otsuki[1,2] and Dieter Vollhardt[1] — [1]Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg — [2]Department of Physics, Tohoku University, Sendai, Japan

To explore the nature of the metallic state near the transition to a Mott insulator, we solve the t-J model with random exchange interaction in $d = \infty$ dimensions. A numerically exact solution is obtained by an extension of the continuous-time quantum Monte Carlo (CT-QMC) method to a model with vector bosonic field coupled to the local spin. It is shown that the paramagnetic solution near the Mott insulator describes an incoherent metal with a residual moment, where the single-particle excitations leads to an additional band separated from the Mott-Hubbard band.

TT 38.12 Wed 12:30 H20

Optical Investigations of the Metal-Insulator Transition in κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Br — •Tomislav Ivek[1,2], Rebecca Beyer[1], Rimma N. Lyubovskaya[3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut za fiziku, Zagreb, Croatia — [3]Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Russian Federation

Due to its fundamental character as well as the promise of practical applications, multiferroicity is at the forefront of investigations in solid state physics. Out of many candidate materials there has been a recent increase of interest in the κ-(BEDT-TTF)$_2$CuX family of quasi-2D organic conductors due to the pronounced dielectric response found in the magnetically-ordered phase. Puzzlingly, in these compounds the infrared vibrational spectroscopy and NMR do not find the charge disproportionation which is a basic prerequisite for electric dipoles.

On the other hand, a related but still unexplored set of mercury-based materials, κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl,Br, shows evidence of charge disproportionation at low temperatures. We present a detailed investigation of the κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Br using infrared spectroscopy and dc transport. Below the metal-insulator transition at 80 K a small transport gap of 20 meV is found within the conducting molecular planes. Far- and mid-infrared spectra are taken between 300 K and 8 K along the three crystallographic axes. We discuss the common optical features as well as more exotic ones compared to the Cu-based κ-materials, particularly temperature dependence of the charge-sensitive vibrational mode $\nu_{27}(B1u)$, in light of recent theoretical descriptions.

TT 38.13 Wed 12:45 H20

Electric-Field Induced Insulator-Metal Transition in α-(BEDT-TTF)$_2$I$_3$ — •Tobias Knoblauch[1], Tomislav Ivek[1,2], Dieter Schweitzer[1], and Martin Dressel[1] — [1]Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut za fiziku, Zagreb, Croatia

Over many decades electric-field induced switching phenomena have been observed in different types of materials, for example, transition metal oxides, inorganic semiconductors as well as organic conductors. In the last mentioned material class, the 2D organic salt α-(BEDT-TTF)$_2$I$_3$ is one of the model systems revealing a metal-insulator phase transition at 136 K in a charge-ordered state. We investigated the switching process in α-(BEDT-TTF)$_2$I$_3$ from the low conducting (charge-ordered) into the high conducting state triggered by a pulsed electric field in a temperature range from 120 to 133 K. The observed nonlinear current-voltage characteristics show negative differential resistance depending on temperature and on the applied electric field. As the underlying physical mechanism is still under con-

sideration, we have performed time-dependent FTIR measurements to track the switching. It gives us, in combination with the steady-state infrared experiments, the possibility to gain more information about the processes responsible for this effect. Here, we also present possible physical models to explain the observed behavior.

TT 38.14 Wed 13:00 H20

Mott Metal-Insulator Transition on Compressible Lattices — •Mario Zacharias[1], Markus Garst[1], and Lorenz Bartosch[2] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Institut für Theoretische Physik, Goethe-Universität, Frankfurt a. M.

In the presence of a coupling to the crystal lattice, the critical properties of the finite temperature Mott end point are drastically altered. While the incompressible Mott transition is analogous to the liquid-gas transition, the compressible Mott transition is a solid-solid transition. Similar as for critical ferroelectrics, the Ising criticality of the electronic system is preempted by an isostructural instability. Long-range shear forces suppress microscopic fluctuations and, thus, the end point is governed by Landau criticality. A hallmark of this effect is the breakdown of Hooke's law of elasticity, i.e. a non-linear strain-stress relation characterized by a mean-field exponent. For the Mott end point of κ-(BEDT-TTF)$_2$X, we predict critical elasticity to dominate in a temperature range $\Delta T^* \simeq 2.5$ K and over a pressure region of $\Delta p \simeq 50$ bar around the end point.