TT 27: Correlated Electrons: Other Materials

Time: Tuesday 9:30–13:00 Location: H 3010

TT 27.1 Tue 9:30 H 3010

Orbital imaging in VO_2 across the insulator to metal transition — •Paulius Dolmantas[1], Chun-Fu Chang[1], Martin Sundermann[1,2], Hlynur Gretarsson[1,2], Marcus Schmidt[1], Maurits W. Haverkort[3], and Arata Tanaka[4] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]DESY/PETRA-III, Hamburg, Germany — [3]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [4]Department of Quantum Matter, Hiroshima University, Japan

Transition metal oxide VO_2 undergoes an metal to insulator transition (MIT) at 340 K from insulating monoclinic phase to a metallic rutile phase. For many decades this MIT in VO_2 has been extensively studied and still is a subject of debate whether it is driven by Mott-Hubbard mechanism or Peierls mechanism. X-ray absorption measurements together with multiplet theory calculations indicated orbital redistribution from almost isotropic in the metallic phase at 373 K to strongly σ orbital polarized at 300 K, suggesting a collaborative Mott-Peierls transition mechanism. Using recently developed X-ray-based orbital-imaging method, we experimentally and directly observe an orbital redistribution across the transition, no theoretical calculations involved. We find that at 20K VO_2 has indeed mainly σ orbital character in the insulating phase. The σ orbital polarization vanishes above the transition. This direct observation of the orbital redistribution across a MIT shall have significant implications for abinitio modeling of metal-insulator transitions.

TT 27.2 Tue 9:45 H 3010

Manipulating the metal-insulator transition in ultrathin oxide films by strain engineering — •Sizhao Huang, Martin Kamp, Fabian Hartmann, Philipp Scheiderer, Judith Gabel, Michael Sing, and Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany

Correlation-induced metal-insulator transitions (MIT) in transition-metal oxides (TMO) have been intensively studied in the past, especially on bulk samples [1]. In TMO films, numerous phenomena can be induced by strain or by reducing the film thickness towards the 2D limit, as, e.g., in $SrVO_3$ (SVO) [2]. In our previous studies on $SrTiO_3$ (STO) capped SVO films, a transition from the Mott insulating state at 6 u.c. to metallic behaviour at 10 u.c. film thickness has been found. In order to further control the MIT transition, we have grown coherently strained SVO thin films on various substrates with different lattice constants by pulsed laser deposition (PLD). Using x-ray photoelectron spectroscopy, reciprocal space mapping and transport measurements, we demonstrate that the MIT in SVO thin films can be fine-tuned by both film thickness and strain, which clears the way for Mottronics applications.

TT 27.3 Tue 10:00 H 3010

The Lorenz ratio as a guide to scattering contributions to Planckian transport — •Fei Sun[1], Simli Mishra[1], Ulrike Stockert[1], Ramzy Daou[2], Naoki Kikugawa[3], Robin S. Perry[4,5], Elena Hassinger[1], Sean A. Hartnoll[6], Andrew P. Mackenzie[1,7], and Veronika Sunko[1,8] — [1]MPI, CPfS, Dresden, Germany — [2]CRISMAT, Caen, France — [3]National Institute for Materials Science, Ibaraki, Japan — [4]University College London, London, UK — [5]ISIS Neutron and Muon Source, UK — [6]University of Cambridge, Cambridge, UK — [7]University of St. Andrews, St. Andrews, UK — [8]University of California Berkeley, USA

A characteristic quantum-mechanical time scale of approximately $\hbar/k_BT$ has been identified recently in both theory and experiment, leading to speculation that it may be the shortest meaningful time in many-body physics. It can be probed in depth by studying the scattering of electrons in solids, however, in metallic oxides, which are among the most studied materials, analysis of electrical transport does not satisfactorily identify the relevant scattering mechanism at high T near room temperature. We employ a contactless optical method to measure thermal diffusivity in two Ru-based layered perovskites, $Sr_3Ru_2O_7$ and Sr_2RuO_4, and use the measurements to extract the dimensionless Lorenz ratio. We show how the analysis of high-T thermal transport can both give important insight into dominant scattering mechanisms, and be offered as a stringent test of theories attempting to explain anomalous scattering.

TT 27.4 Tue 10:15 H 3010

Ferromagnetism in epitaxial $Ca_{1-x}Sr_xIrO_3$ thin films grown by metal-organic aerosol deposition — •Robert Gruhl, Ludwig Scheuchenpflug, Robin Heumann, and Philipp Gegenwart — Experimentalphysik VI, Universität Augsburg, Germany

$SrIrO_3$ is a paramagnetic semimetal with strong spin-orbit coupling which can give rise to various interesting physical states [1]. The isostructural and isoelectric perovskite phase of $CaIrO_3$ has very similar properties but a significantly smaller unit cell [2]. This enables a tuning of the lattice parameter over a wide range by chemical doping in the form of $Ca_{1-x}Sr_xIrO_3$.

Suprisingly small amounts of Calcium lead to a ferromagnetic phase in the investigated fully strained thin films as indicated by an emergent anomalous Hall effect. This behaviour is accopanied by an unusual increase in the out-off-plane lattice parameter.

Epitaxial thin films of $Sr_{1-x}Ca_xIrO_3$ are deposited on STO(001) substrates by metal-organic aerosol deposition, which conveniently allows to grow thin films with varying chemical compositions, since in contrast to PLD no target is required. The structural properties of the samples are investigated by x-ray diffraction and TEM imaging. The electronic and magnetic properties are studied by Hall- and magnetoresistance as well as magnetization mesasurements.

[1] K. Kleindienst *et al.*, Phys. Rev. B 98, 115113 (2018).
[2] A. Biswas *et al.*, J. Appl. Phys. 21, 195305 (2015).

TT 27.5 Tue 10:30 H 3010

Dynamics of exciton-polaritons in optically driven ZnO nano-particles — Andreas Lubatsch[1] and •Regine Frank[2,3] — [1]Physikalisches Institut, Rheinische Friedrich Wilhelms Universität Bonn — [2]College of Biomedical Sciences, Larkin University, Miami, Florida, USA — [3]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain

We implement externally excited ZnO Mie resonators in a framework of a generalized Hubbard Hamiltonian to investigate the lifetimes of excitons and exciton-polaritons outthermodynamical equilibrium. Our results are derived by a Floquet-Keldysh-Green's formalism with Dynamical Mean Field Theory (DMFT) and a second order iterative perturbation theory solver (IPT). We find polaritons that result from the Fano resonance in the sense of coupling of the continuum of the LDOS to the ZnO resonator with lifetimes between 0.6 ps and 1.45 ps. Our results are compared to rescent experiments of ZnO polariton lasers and to ZnO random lasers.

[1] A. Lubatsch, R. Frank, Appl. Sci. 10 (2020) 1836
[2] A. Lubatsch, R. Frank, Symmetry 11 (2019) 1246
[3] T.-C. Lu, et. al., Opt. Express 20 (2010) 5530

TT 27.6 Tue 10:45 H 3010

Superconductivity and Mottness in Organic Charge Transfer Materials — Henri Menke[1,2], Marcel Klett[1], Kazushi Kanoda[1,3], Antoine Georges[4], Michel Ferrero[5], and •Thomas Schäfer[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]University of Erlangen-Nürnberg — [3]University of Stuttgart — [4]Center for Computational Quantum Physics, Flatiron Institute — [5]CPHT, CNRS, École Polytechnique, Palaiseau

The phase diagrams of organic superconductors assemble a plethora of fundamental phenomena of strongly correlated systems in two dimensions. We analyze a minimal model for these compounds, the Hubbard model on an anisotropic triangular lattice, by means of cutting-edge quantum embedding methods, respecting the lattice symmetry. We determine the crossover from a Fermi liquid to a Mott insulator by momentum-selective destruction of the Fermi surface reminiscent of a pseudogap. In the immediate vicinity of the metal-insulator crossover we demonstrate the existence of unconventional superconductivity by directly entering the symmetry-broken phase. Our results are in remarkable agreement with experimental phase diagrams of κ-organics for which we motivate future spectroscopic studies of hot and cold spots.

TT 27.7 Tue 11:00 H 3010

Increase of resistance noise across the Mott transition —

•Tim Thyzel[1], Jens Müller[1], Harald Schubert[1], Michael Lang[1], Takahiko Sasaki[2], and Hiroshi Yamamoto[3] — [1]Institute of Physics, Goethe-Universität Frankfurt, Frankfurt (Main), Germany — [2]Institute of Materials Research, Tohoku University, Sendai, Japan — [3]Institute for Molecular Science, Graduate University for Advanced Studies, Okazaki, Japan

The Mott metal-insulator transition, being driven by the Coulomb interaction between crystal electrons, is of fundamental interest in the field of strongly correlated electron systems. Using the quasi-two-dimensional organic metal κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl as a model compound for the Mott transition, we examined the slow dynamics in the charge transport by means of fluctuation spectroscopy.

This method reveals a marked, smooth increase in the low-frequency resistance noise as the system is tuned from its insulating to the metallic phase by changing the bandwidth using hydrostatic pressure. Our finding contributes to the discussion about the nature of finite-temperature Mott criticality [1,2], and raises questions about the role of disorder in the charge dynamics near a Mott instability.

In addition to bandwidth control, we make use of the field effect for carrier doping of a system close to the Mott transition [3]. This will allow us to explore the changes in charge dynamics without modifying the band structure.

[1] Gati, Science Adv. 2, e1601646
[2] Hartmann, Phys. Rev. Lett. 114, 216403
[3] Yamamoto, Nat. Commun. 4, 2379

15 min. break

TT 27.8 Tue 11:30 H 3010

Influence of chemical/structural modifications in layered organic salts κ-(BEDT-TTF)$_2$X near the Mott transition probed by magnetic quantum oscillations. — •Shamil Erkenov[1,2], Florian Kollmannsberger[1,2], Werner Biberacher[1], Ilya Sheikin[3], Toni Helm[4], Natalia Kushch[1], Rudolf Gross[1,2], and Mark Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]Laboratoire National des Champs Magnétiques Intenses, Grenoble, France — [4]Hochfeld-Magnetlabor Dresden, HZDR, Dresden, Germany

One of the prominent systems for studying Mott metal-insulating transition (MIT) are organic salts κ-(BEDT-TTF)$_2$X. These salts have different electronic ground states, determined by electronic corelations U/t and spin frustration ratio t'/t, which can be tuned by a pressure or via chemical/structural modifications, such as anion substitution or ordering of the BEDT-TTF ethylene endgroups. It was believed that chemical/structural modifications act similarly to physical pressure and change electronic state of the system via changing U/t. However, first-principles band-structure calculations [1] suggest that anion substitution in κ salts influences the ground state primarily through the change of the ratio t'/t rather than U/t. Here we report on comparative studies of magnetic quantum oscillations in the κ salts, with X = Cu(NCS)$_2$, Cu[N(CN)$_2$]Y (Y=Cl, Br) and Cu$_2$(CN)$_3$ to trace the correlations between the anion substitution and the mentioned ratios.

[1] T. Koretsune and C. Hotta, Phys. Rev. B **89**, 045102 (2014).

TT 27.9 Tue 11:45 H 3010

Field-driven tuning of magnetic excitations in the van der Waals compound CuCrP$_2$S$_6$ (CCPS) — •Joyal John Abraham[1,2], Sebastian Selter[1], Yuliia Shemerliuk[1], Saicharan Aswartham[1], Bernd Büchner[1,3], Vladislav Kataev[1], and Alexey Alfonsov[1] — [1]Leibniz IFW Dresden, D-01069 — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01069 — [3]Institute for Solid State and Materials Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, D-01062

High-frequency ESR was performed on a single crystal of CCPS. The magnetic Cr^{3+} ions forming ferromagnetic layers are diluted with non-magnetic Cu^{1+} ions which makes it interesting compared to other members in the metal-P$_2$S$_6$ family. The adjacent layers are coupled antiferomagnetically. We have found that at 300 K, CCPS behaves as a paramagnet with almost spin-only g-factors showing a small anisotropy. Below $T \approx$ 200-250 K, the ESR line shifts from the paramagnetic position indicating the presence of a broad range of short-range spin-spin correlations. In the ordered state below $T_N = 30$ K, we observed two excitation gaps and a spin flop at 0.43 T. Remarkably, at stronger magnetic fields a crossover from the antiferromagnetic (AFM) resonance modes to the FM modes, unexpected for a canonical antiferromagnet takes place. Application of the linear spin wave theory enabled us to quantify the exchange (A) and anisotropic constants. The value of A is found to be comparable to the value of the easy-plane uniaxial anisotropy, which explains such an unusual AFM-FM crossover.

TT 27.10 Tue 12:00 H 3010

^{31}P NMR studies of quasi-two-dimensional magnetic correlations in ACrP$_2$S$_6$ (A= Cu, Ag) — •Saramgi Chencheriparambil Sivan[1,2], Ranjith Kumar Kizhake Malayil[1], Lukas Prager[1], Saicharan Aswartham[1], Bernd Büchner[1,2], and Hans-Joachim Grafe[1] — [1]Leibniz IFW Dresden, D-01069 — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01069

The AA'P$_2$S$_6$ (A, A' = transition metal ions) family of quasi-two-dimensional van der Waals materials has proven to be a model system for low-dimensional magnetism. These materials provide an ideal platform to study the Hamiltonians of fundamental magnetism models, including the Ising, XY, and Heisenberg models. Here we present detailed ^{31}P NMR measurements on single-crystal samples of ACrP$_2$S$_6$. The high-temperature single narrow NMR line shows a splitting at about 160 K for CuCrP$_2$S$_6$, which is due to the antiferroelectric transition, while a *pake−doublet* NMR spectrum is observed for AgCrP$_2$S$_6$ at room temperature. In CuCrP$_2$S$_6$, we observed further line splitting below 30 K, reflecting the antiferromagnetic (AFM) order. At $T_N = 30$ K, the NMR spin-lattice relaxation rate T_1^{-1}(T) in CuCrP$_2$S$_6$ shows a sharp peak due to the critical fluctuations. The temperature dependence of $(T_1T)^{-1}$ shows a broad maximum at about 60 K and a critical enhancement at T_N. T_N are anisotropic near the critical regime. AgCrP$_2$S$_6$ exhibits AFM order at 20 K, as evidenced by the clear splitting of the NMR spectra and the divergence of T_1^{-1}(T) at T_N. In contrast to CuCrP$_2$S$_6$, the temperature dependence of $(T_1T)^{-1}$ shows only a critical enhancement around T_N without a broad anomaly.

TT 27.11 Tue 12:15 H 3010

Elastoresistance of the itinerant antiferromagnet Ca$_{1-x}$Sr$_x$Co$_{2-y}$As$_2$: Analysis of different symmetry channels — •Teslin Rose Thomas, N. S. Sangeetha, Sven Graus, Max Brückner, Andreas Kreyssig, and Anna E. Böhmer — Lehrstuhl für Experimentalphysik IV, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum

It is becoming common to study correlated electron systems using elastoresistance, the change in electrical resistance under strain. An interesting aspect of this technique is the possibility of applying symmetry-selective strain to the system under investigation. In this study, we present the method of uniaxial/biaxial elastoresistance and how it can be applied to study various symmetry channels. The method is applied to the itinerant antiferromagnet Ca$_{1-x}$Sr$_x$Co$_{2-y}$As$_2$ that shows a collapsed-to-uncollapsed tetragonal structural crossover and interesting magnetic orderings upon Sr substitution [1, 2]. We observe prominent and diverse signals in the different symmetry channels, especially a large A$_{1g}$ (non-symmetry breaking) elastoresistance.

We acknowledge support from the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] N. S. Sangeetha et al., Phys. Rev. Lett. 119 (2017) 257203
[2] Bing Li et al., Phys. Rev. B 100 (2019) 024415

TT 27.12 Tue 12:30 H 3010

Phases and Exotic Phase Transitions of a Two-Dimensional Su-Schrieffer-Heeger Model — •Anika Götz[1], Martin Hohenadler[1], and Fakher Assaad[1,2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany

We study a Su-Schrieffer-Heeger electron-phonon model on a square lattice with auxiliary-field quantum Monte Carlo simulations. Adding a symmetry-allowed interaction permits analytical integration over the phonons at the expense of discrete Hubbard-Stratonovich fields with imaginary-time correlations. We investigate the phase diagram at the O(4)-symmetric point as a function of hopping t and phonon frequency ω_0. For $t = 0$, where electron hopping is boson-assisted, the model maps onto an unconstrained $\mathbb{Z}_2$ gauge theory. A key quantity is the emergent effective flux per plaquette, which equals π in the assisted-hopping regime and vanishes for large t. Phases in the former regime can be understood in terms of instabilities of emergent Dirac fermions. Our results support a direct and continuous transition between a $(\pi, 0)$ valence bond solid (VBS) and an antiferromagnetic (AFM) phase with increasing ω_0. By increasing the electronic interaction the critical

phonon frequency can be lowered, driving the transition to a first order one. In addition the role of doping away from half-filling is studied. For large t and small ω_0, we find finite-temperature signatures of a previously reported (π, π) VBS ground state related to a nesting instability. With increasing ω_0, AFM order again emerges.

TT 27.13 Tue 12:45 H 3010

Study of M_3O_{12} trimers in transition metal cluster Mott insulators — •Vaishnavi Jayakumar[1] and Ciarán Hickey[1,2,3] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland — [3]Centre for Quantum Engineering, Science and Technology, University College Dublin, Dublin 4, Ireland

Recent progress in the synthesis of transition metal compounds which are potential cluster Mott insulators provides an opportunity to study these materials more closely. In this work, we use exact diagonalization techniques to study the series of 12L hexagonal perovskites $Ba_4NbM_3O_{12}$ and consider different fillings of $3d$ to $5d$ transition-metal M ions. These perovskites consist of linear face-sharing M_3O_{12} trimer clusters, and can be best described as lying between the localized-electron picture and molecular orbital picture. We find that the local effective degrees of freedom and other ground-state properties can be shown to be due to an interplay between strong correlations and hopping within the clusters. In addition, we also perform an exhaustive study of all possible fillings on these trimer clusters. Our results show, for example, that there can exist ground state degeneracies that are due to cluster or orbital point group symmetries, in parameter regimes where we might conventionally expect to see a unique ground state. We use our study to hence propose ground state properties and phase diagrams for materials that are likely to be synthesized in the future.