TT 3: Correlated Electrons: Electronic Structure Calculations

Time: Monday 9:30–10:45 Location: HSZ/0103

TT 3.1 Mon 9:30 HSZ/0103

Electronic structure, effective model and electron correlation in Ruddlesden-Popper Cobalt Oxychloride — •Xiaolong Feng[1], Yang Zhang[2,3], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA — [3]Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee 37996, USA

Recent advances in Ruddlesden-Popper(RP)-layered nickelates have revealed a remarkable superconducting transition above the boiling point of liquid nitrogen under high pressure. Here, we report a theoretical investigation of RP cobalt oxychloride, which shows a correlation-driven metal-insulator transition. Strong hybridization between Co-d orbitals and O-p orbitals is identified close to the Fermi level. Upon incorporating enhanced electronic correlations, the Co-d orbital emerges as the dominant component at the Fermi level with partial filling. To further explore the ground state, we construct a minimal effective model via Wannier downfolding, capturing the essential physics of the system. Notably, our results predict an insulator-metal transition under high pressure, positioning RP cobalt oxychloride as a compelling candidate for studying correlated transition metal compounds with potential magnetism and superconductivity.

TT 3.2 Mon 9:45 HSZ/0103

Imaging the $3d$ orbitals in V_2O_3 across the AFI-PM-PI transitions — •Paulius Dolmantas[1], Chun-Fu Chang[1], Martin Sundermann[1,2], Hlynur Gretarsson[2], Jonathan Denlinger[3], Maurits Haverkort[4], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]DESY, Hamburg, Germany — [3]ALS, Berkeley, USA — [4]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

V_2O_3 exhibits a rich phase diagram in which the transitions between the antiferromagnetic insulating (AFI), paramagnetic metallic (PM) and paramagnetic insulating (PI) phases are all 1^{st} order. The presence of c-axis V-V dimers in the crystal structure is the reason for proposing the standard model for V_2O_3 in which a_{1g}-a_{1g} molecular singlets are formed, leaving each V ion with an S=1/2 electron to generate the complex phase diagram. Numerous *ab-initio* electronic structure calculations and spectroscopy studies have been carried out to determine the mechanism of the phase transitions, with contradicting results. The main problem underlying this issue is that the actual valence charge density in V_2O_3 has not yet been determined with sufficient reliability, a quantity that forms the very basis for modeling the properties. Here we utilized a newly developed experimental method with which we can make a direct image of the active orbital. The method is non-resonant inelastic X-ray scattering using an s-core level. Our experimental results unveiled that the a_{1g}-a_{1g} molecular singlets have not materialized and that instead, subtle changes changes in the orbital occupations across the transitions must be considered.

TT 3.3 Mon 10:00 HSZ/0103

$Ni_{1/3}NbS_2$: A correlated impurity-lattice with Ni^{2+} in a metallic Van der Waals magnet — •Sheng-Huai Chen[1], Chun-Fu Chang[1], Yu-Chih Ku[2,3], Po-Yu Cho[2], Chang-Yang Kuo[2,3], Marcus Schmidt[1], Antoine Maignan[4], Atsushi Hariki[5], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Germany — [2]Natl. Synchrotron Radiation Research Center, Taiwan — [3]Dep. of Electrophysics, Natl. Yang Ming Chiao Tung University, Taiwan — [4]CRISMAT, Normandie Univ., CNRS, France — [5]Dep. of Phys. and Electronics, Osaka Metropolitan University, Japan

Ni-intercalated NbS_2 has attracted considerable attention as a chiral metallic van der Waals magnet that couples helical antiferromagnetism to a conducting Nb-4d/S-3p host, exhibiting current-driven spin-texture control, and showing pocket-selective Fermi surface doping. Our objective is to investigate the specific role of the Ni ions in here. In particular, we would like to know as to what extent electron correlations play a role, and if so, what the actual valence and electronic configurations the Ni has. By combining Ni $L_{2,3}$ XAS, Ni $2p$ XPS, valence band and resonant PES with material-specific DFT+DMFT calculations, we establish that the Ni has a strongly correlated local electronic structure with the Ni^{2+} ($3d^8$) as the main configuration. The NiS_6 octahedra thus set the existence and scale of the local moment and single-ion anisotropy that are the ingredients for the helical state. The interplay between the correlated Ni states with the dispersing bands forming the Fermi surface is the subject of ongoing study.

TT 3.4 Mon 10:15 HSZ/0103

Origin of orbital and magnetic transitions in rare-earth perovskites — •Xuejing Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Supercomputing Centre, Forschungszentrum Jülich, 52425 Jülich, Germany

Strongly-correlated transition-metal oxides are characterized by complex phase diagrams, which result from the interplay of orbital, charge, lattice and spin degrees of freedom. Recently, we introduced an efficient scheme to investigate these phenomena [1-3]. It combines the LDA+DMFT method with a analysis scheme based on the decomposition of the order parameter into its irreducible components. Thanks to this approach, we could explain the origin of the inversion of orbital and magnetic order observed with increasing rare-earth (R) radius in the t_{2g}^2 series RVO_3 [3]. Here we present results for these as well as for other systems.

[1] X. J. Zhang, E. Koch, E. Pavarini, PRB **105** (2022) 115104
[2] X. J. Zhang, E. Koch, E. Pavarini, PRB **106** (2022) 115110
[3] X. J. Zhang, E. Koch, E. Pavarini, PRL **135** (2025) 026508

TT 3.5 Mon 10:30 HSZ/0103

Real-frequency DMFT for multi-orbital models with the neural network configuration interaction impurity solver — •Alexander Kowalski[1], Philipp Hansmann[2], Giorgio Sangiovanni[1], and Adriana Pálffy[1] — [1]Institute for Theoretical Physics and Astrophysics, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The numerical solution of an auxiliary Anderson Impurity Model is usually the most resource-intensive part of the dynamical mean-field treatment of strongly correlated lattice models. Among the variety of approaches with different trade-offs that have been developed, the problem with exact diagonalization is that the exponential scaling of the Hilbert space constrains it to describing the infinite bath in terms of only a small finite number of sites. Selected Configuration Interaction (CI) methods try to achieve more favorable scaling by performing an a priori restriction of the basis used for diagonalization to try to capture only the most important subspace of the desired size. Neural networks have been shown to be remarkably suitable for performing the CI basis selection [1] and we have previously previewed the integration of such a CI algorithm as impurity solver in DMFT. Further developments since then have allowed us to do DMFT calculations with self-consistency directly on the real frequency axis for multi-orbital models with numbers of bath sites well beyond the reach of exact diagonalization.

[1] P. Bilous, L. Thirion, H. Menke, M. W. Haverkort, A. Pálffy, P. Hansmann, Phys. Rev. B 111, 035124 (2025)