TT 39: Correlated Electrons: Charge Order

Time: Friday 11:15–13:15 Location: H23

TT 39.1 Fri 11:15 H23

Stripe discommensuration and spin dynamics of charge and spin stripe ordered $Pr_{3/2}Sr_{1/2}NiO_4$ — •Avishek Maity[1], Rajesh Dutta[2,3], and Werner Paulus[4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85747 Garching, Germany — [2]Institut für Kristallographie, RWTH Aachen Universität, 52066 Aachen, Germany — [3]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), 85747 Garching, Germany — [4]Institut Charles Gerhardt Montpellier, Université de Montpellier, 34095 Montpellier, France

Magnetic excitations in the charge and spin stripe ordered phases of La-based 214-nickelates have been vigorously explored using inelastic neutron scattering (INS) studies. In view of so far reported two-dimensional antiferromagnetic nature, out-of-plane interaction is not generally expected in 214-nickelates. Here we will present our results on the magnetic excitations of $Pr_{3/2}Sr_{1/2}NiO_4$, with stripe incommensurability $\epsilon = 0.4$, showing a very compelling evidence for the presence of a sizable out-of-plane interaction ($J_\perp \sim 2.2$ meV) manifesting a symmetrical outward shift of the spin wave dispersion from the antiferromagnetic zone center. Our linear spin wave calculation using an unconventional three-dimensional model of discommensurated spin stripe (DCSS) unit for $\epsilon = 0.4$ could explicitly show such outward shift results from the overlap of a mode originating exclusively from the out-of-plane interaction. Our study suggests that a careful consideration of the out-of-plane interaction is necessary in the stripe discommensurated 214-nickelates.
[1] A. Maity et al., PRL 124, 147202 (2020).

TT 39.2 Fri 11:30 H23

Quantum oscillations in the Kagome superconductor CsV_3Sb_5 — •Anmol Shukla[1], Liran Wang[1], Frédéric Hardy[1], Amir-Abbas Haghighirad[1], Mingquan He[2], Wei Xia[3], Yanfeng Guo[3], and Christoph Meingast[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Low Temperature Physics Lab, College of Physics & Center of Quantum Materials and Devices, Chongqing University, Chongqing 401331, China — [3]School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China

The recently discovered layered Kagome metals AV_3Sb_5 (A = K, Rb, Cs) exhibit a unique combination of nontrivial band topology, competing for the charge- and superconducting orders with clear signatures of electron correlations. Using magnetization, resistivity, thermal expansion, magnetostriction and heat capacity, we have investigated the normal- and superconducting-state properties of single crystals of the kagome superconductor CsV_3Sb_5. The magnetization and magnetostriction data show clear signatures of quantum oscillations with at least two distinct frequencies. These are much less evident in the heat capacity. Combining the results from these thermodynamic probes and transport measurement, we discuss the nature of the Fermi surface and the interplay between the charge order and superconductivity.

TT 39.3 Fri 11:45 H23

Statistical learning of engineered topological phases in the Kagome superlattice of AV_3Sb_5 — Thomas Mertz, •Paul Wunderlich, Shinibali Bhattacharyya, Francesco Ferrari, and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany

Recently, the kagome metals AV_3Sb_5 (A = K,Rb,Cs) have gained intense research interest, as they display a wide spectrum of exotic topological properties, in addition to superconductivity, charge, orbital momentum and spin density waves. Motivated by a plethora of experimental evidence for unconventional charge orders in the enlarged (2×2) unit-cell of the vanadium based kagome metals, we investigate the type of topological phases that can manifest within the electronic parameter space of such kagome superlattices. Unlike conventional theoretical approaches, we employ a recently introduced statistical method capable of constructing topological models for any generic lattice, in an unbiased way without prior knowledge of its phase diagram. By extracting physically meaningful information from large datasets of randomized hopping parameters for the kagome superlattice, we find possible real-space manifestations of charge and bond modulations and associated flux patterns for different topological classes. Our results agree with contemporary theoretical propositions and experimental observations for the AV_3Sb_5 family. Simultaneously, we predict new higher-order topological phases that may be realized by appropriately manipulating the currently known systems.

TT 39.4 Fri 12:00 H23

High-pressure IR investigations unveil modifications in the electronic structure of the superconducting Kagome metal CsV_3Sb_5 — •Maxim Wenzel[1], Yuk T. Chan[1], Brenden R. Ortiz[2,3], Stephen D. Wilson[3], Martin Dressel[1], Alexander A. Tsirlin[4], and Ece Uykur[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]California Nanosystems Institute, University of California Santa Barbara, Santa Barbara, CA, 93106, United States — [3]Materials Department, University of California Santa Barbara, Santa Barbara, CA, 93106, United States — [4]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

The non-magnetic Kagome metal series AV_3Sb_5 with A = K, Cs, or Rb is known for the coexistence of charge-density-wave and superconducting orders at low temperatures. Previously, the tunability of both orders has been investigated extensively via high-pressure transport studies; however, the pressure-induced modifications of the electronic band structure, especially the position of the saddle points, remain the subject of current research. While theoretical studies present conflicting suggestions regarding the pressure effects on the band structure, it has been shown that the interband optical transitions are highly sensitive to the position of the saddle points and hence, can probe them experimentally. Therefore, we performed high-pressure infrared studies on the model compound CsV_3Sb_5 at room temperature to trace the behavior of the interband optical transitions up to 17 GPa.

TT 39.5 Fri 12:15 H23

Charge-density waves in Kagome-lattice extended Hubbard models at the van Hove filling — •Francesco Ferrari[1], Federico Becca[2], and Roser Valentí[1] — [1]Goethe University, Frankfurt am Main, Germany — [2]University of Trieste, Trieste, Italy

The Hubbard model on the kagome lattice is presently often considered as a minimal model to describe the rich low-temperature behavior of AV_3Sb_5 compounds (with A=K, Rb, Cs), including charge-density waves (CDWs), superconductivity, and possibly broken time-reversal symmetry. We investigate, via variational Jastrow-Slater wave functions, the properties of its ground state when both onsite U and nearest-neighbor V Coulomb repulsions are considered at the van Hove filling. Our calculations reveal the presence of different interaction-driven CDWs and, contrary to previous renormalization-group studies, the absence of ferromagnetism and charge- or spin-bond order. No signatures of chiral phases are detected. Remarkably, the CDWs triggered by the nearest-neighbor repulsion possess charge isproportionations that are not compatible with the ones observed in AV_3Sb_5. As an alternative mechanism to stabilize charge-bond order, we consider the electron-phonon interaction, modeled by coupling the hopping amplitudes to quantum phonons, as in the Su-Schrieffer-Heeger model. Our results show the instability towards a tri-hexagonal distortion with 2x2 periodicity, in a closer agreement with experimental findings.

TT 39.6 Fri 12:30 H23

Chalcogenic orbital density waves in the weak- and strong-coupling limit — •Adam Kłosiński[1], Andrzej M. Oleś[2,3], Clio Efthimia Agrapidis[1], Jasper van Wezel[4], and Krzysztof Wohlfeld[1] — [1]University of Warsaw, Warsaw, Poland — [2]Jagiellonian University, Krakow, Poland — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]University of Amsterdam, Amsterdam, The Netherlands

Stimulated by recent works highlighting the indispensable role of Coulomb interactions in the formation of helical chains and chiral electronic order in the elemental chalcogens, we explore the p-orbital Hubbard model on a one-dimensional helical chain. By solving it in the Hartree approximation we find a stable ground state with a period-3 orbital density wave. We establish that the precise form of the emerging order strongly depends on the Hubbard interaction strength. In the strong-coupling limit, the Coulomb interactions support an orbital density wave that is qualitatively different from that in the weak-

coupling regime. We identify the phase transition separating these two orbital ordered phases and show that realistic values for the interorbital Coulomb repulsion in elemental chalcogens place them in the weak-coupling phase, in agreement with observations of the order in the elemental chalcogens.

TT 39.7 Fri 12:45 H23

Understanding the transition from metal to Hund's insulator in $CaFeO_3$ — •Maximilian Merkel and Claude Ederer — Materials Theory Group, ETH Zürich, Switzerland

Materials where strong correlations are caused by the Hund's interaction have recently attracted a lot of attention. In some cases, a dominant Hund's interaction can even lead to the emergence of a charge-disproportionated insulating (CDI) or "Hund's insulating" state. One example is the perovskite transition-metal oxide $CaFeO_3$ (CFO), which exhibits a transition from metal to Hund's insulator around room temperature. This transition couples to a structural distortion that creates alternating large and small FeO_6 octahedra, leading to two inequivalent Fe sites with nominal Fe^{5+} and Fe^{3+} charge states. We study CFO using density functional theory (DFT) and dynamical mean-field theory (DMFT). To characterize the CDI state, we first apply DMFT to a five-orbital Hubbard model applicable to CFO and demonstrate the emergence of the CDI phase here [1]. We then investigate the energetics of the transition using fully self-consistent DFT+DMFT calculations. We discuss the ligand-hole character of the charge disproportionation due to the zero or even negative charge-transfer energy. Our calculations show that both structural and electronic properties of the CDI state are well described within DFT+DMFT but also that the subtle interplay of several effects represents a big challenge for any quantitative, predictive theory.

[1] M. E. Merkel and C. Ederer, Phys. Rev. B 104, 165135 (2021)

TT 39.8 Fri 13:00 H23

Reinvestigating the metallic region of the half-filled Hubbard Holstein model — Sam Mardazad[1], Martin Grundner[1], Ulrich Schollwöck[1], Adrian Kantian[2], Thomas Köhler[3], and •Sebastian Paeckel[1] — [1]Department of Physics, Arnold Sommerfeld Center of Theoretical Physics, University of Munich, Germany — [2]Institute of Photonics and Quantum Sciences, Heriot-Watt University, Edinburgh, UK — [3]Department of Physics and Astronomy, Uppsala University, Sweden

The one-dimensional Hubbard-Holstein model is the paradigmatic system to study the interplay between strongly correlated electrons and dispersionless lattice vibrations. Particularly, the intermediate regime of competing interactions has been heavily debated and only with the advent of powerful numerical techniques such as density-matrix renormalization group (DMRG) or advanced quantum Monte Carlo (QMC), the realization of an intermediate metallic phase has been established. However, these early studies are characterized by significant truncations of the phononic Hilbert spaces. Here, we exploit recent advances in the efficient representation of large local Hilbert spaces to re-examine the phase diagram by large-scale DMRG calculations, focussing on the regime of competing, strong interactions. This allows us to systematically study the complex competition between correlations, overcoming previous limitations.