

TT 13: Kagome Systems

Time: Monday 15:00–18:15

Location: H 3010

TT 13.1 Mon 15:00 H 3010

Investigation of the charge density wave in single crystal CsV₃Sb₅ under hydrostatic pressure — FABIAN STIER¹, AMIR HAGHIGHIRAD³, TOBIAS RITSCHER¹, CHANDRA SHEKHAR², CLAUDIA FELSER², JOCHEN GECK¹, and MATTHIEU LE TACON³ — ¹IFMP, TU Dresden, Germany — ²MPI CPFS, Dresden, Germany — ³IQMT, KIT, Karlsruhe, Germany

The kagome materials AV₃Sb₅ (A = K, Rb, Cs) show a nontrivial electronic topology, exhibit unconventional superconductivity (SC) and charge-density-wave (CDW) order. We investigated the CDW in two different sample batches of CsV₃Sb₅ using x-ray diffraction as a function of hydrostatic pressure and temperature at the ID15B Beamline at the ESRF. Samples from both batches were loaded in the same diamond anvil cell (DAC) to ensure equal experimental conditions. Near ambient pressure, both sample batches exhibit the previously reported 2x2x2 and 2x2x4 CDW. The order in which these phases occur with decreasing temperature is reversed in one sample batch with respect to the other. Increasing the pressure at low temperature yields a new CDW order, which is the same in both batches. The critical pressures at which this new CDW phase appears and finally vanishes again, correspond well to the previously reported anomalies in the pressure dependence of the SC transition temperature. At low temperature and higher pressures the samples show another transient transition from the hexagonal unit cell to a monoclinic cell. Using our experimental results in combination with DFT calculations we will discuss the pressure effects on the electronic structure and the superconductivity.

TT 13.2 Mon 15:15 H 3010

Unconventional superconductivity on the kagome lattice — BRIAN MØLLER ANDERSEN, SOFIE CASTRO HOLBEAK, MORTEN HOLM CHRISTENSEN, and ANDREAS KREISEL — Niels Bohr Institute, University of Copenhagen, DK-2200 Copenhagen, Denmark

Recent developments have focussed research on unusual electronic orders on the kagome lattice. This is evident mainly from the discovery of CDW phases and superconductivity in the AV₃Sb₅ (A:K, Rb, Cs) metals. We discuss the general expected form of superconductivity on the kagome lattice from charge- and spin-fluctuations. Some discussion will also be included on the potential role of orbital-selective phonons on the nature of superconductivity in the specific AV₃Sb₅ compounds. The second part of the talk addresses disorder on the kagome lattice. Surprisingly, unconventional superconductivity with sign-changing order parameters are remarkable robust to point-like nonmagnetic disorder. We demonstrate this effect by explicit calculations of bound states and Tc-suppression rates. The origin of the robustness is tied to the particular sublattice interference present for the electronic states on the kagome lattice.

TT 13.3 Mon 15:30 H 3010

Non-equilibrium carrier dynamics of the CsV₃Sb₅ kagome metal — KAI FRISCH¹, NIKLAS HOFMANN¹, LEONARD WEIGL¹, JOHANNES GRADL¹, BRENDEN ORTIZ², ANDREA CAPA SALINAS³, STEPHEN WILSON³, and ISABELLA GIERZ¹ — ¹University of Regensburg — ²Oak Ridge national Lab — ³University of California, Santa Barbara

The V planes in AV₃Sb₅ (A=K, Rb, Cs) form a kagome lattice, resulting in a peculiar electronic structure with coexisting Dirac cones and flat bands [1]. The compounds exhibit a possibly chiral CDW below ~ 90 K and become superconducting below ~ 3 K consistent with predictions from a kagome Hubbard model at van Hove filling [2]. We use time- and angle-resolved photoemission spectroscopy to study the non-equilibrium carrier dynamics of CsV₃Sb₅ in its metallic room temperature phase. We extract the transient electronic temperature of the carriers and interpret the cooling dynamics in terms of strongly coupled optical phonons. Our results shed light onto the coupling between electrons and phonons in kagome metals, relevant for unraveling the mechanism behind the different exotic ground states.

[1] Phys. Rev. Materials, 3 094407 (2019)

[2] Phys. Rev. B 86, 121105(R) (2012)

TT 13.4 Mon 15:45 H 3010

Order-by-disorder charge density wave condensation at $q = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ in kagome metal ScV₆Sn₆ — ALASKA SUBEDI —

CPHT, CNRS, Ecole Polytechnique, IP Paris, Palaiseau, France

The recent discovery of a charge density wave order at the wave vector $P (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ in the kagome metal ScV₆Sn₆ has created a mystery because subsequent theoretical and experimental studies show a dominant phonon instability instead at another wave vector $H (\frac{1}{3}, \frac{1}{3}, \frac{1}{2})$. Here, I discuss the results of first principles total energy calculations that were used to map out the landscape of the structural distortions due to the unstable phonon modes at H , $L (\frac{1}{2}, 0, \frac{1}{2})$, and P present in this material. In agreement with previous results, I find that the distortions due to the H instability cause the largest gain in energy relative to the parent structure, followed in order by the L and P instabilities. However, only two distinct structure occur due to this instability, which are separated by 6 meV/f.u. The instability at L results in three distinct structures separated in energy by 5 meV/f.u. In contrast, six different distorted structures are stabilized due to the instability at P , and they all lie within 2 meV/f.u. of each other. Hence, despite a lower energy gain, the condensation at P could be favorable due to a larger entropy gain associated with the fluctuations within a manifold with larger multiplicity via the order-by-disorder mechanism.

TT 13.5 Mon 16:00 H 3010

⁵¹V Nuclear Magnetic Resonance as a Local Probe for the Charge Ordered Kagome System ScV₆Sn₆ — ROBIN GUEHNE, JONATHAN NOKY, CHANDRA SHEKHAR, MAIA G. VERGNIORY, MICHAEL BAENITZ, and CLAUDIA FELSER — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Intermetallic compounds featuring Kagome lattice planes have lately attracted immense attention as platforms that provide the opportunity to study a diversity of topological features, like van Hove singularities, Dirac cones, and correlated flat bands. Some of these materials show long-range charge order. This is the case for the Vanadium based Kagome metal ScV₆Sn₆ that undergoes a charge density wave (CDW) transition around 96 K. The origin of this transition is still under debate, even more so the properties of the CDW phase, such as related to chirality of the charge order or hidden magnetism [1]. We use ⁵¹V nuclear magnetic resonance (NMR) to investigate the CDW phase transition from a local point of view. Aided by density functional theory (DFT), NMR allows us to separate the chemistry from electronic properties and to identify the CDW fingerprint encoded in the NMR shift and relaxation amid the structural phase transition that manifests in the electric quadrupole interaction. In the presentation we will give an overview of the results and discuss potential implications.

[1] C. Yi, X. Feng, P. Yanda, S. Roychowdhury, C. Felser, C. Shekhar, arXiv:2305.04683 (2023)

TT 13.6 Mon 16:15 H 3010

Charge carrier dynamics of kagome metals GdMn₆Sn₆ and TbMn₆Sn₆ probed by transient reflectivity — MARCOS VINICIUS GONCALVES FARIA^{1,2}, ALEXEJ PASHKIN¹, STEPHAN WINNERL¹, HECHANG LEI³, QI WANG³, MAXIM WENZEL⁴, MANFRED HELM^{1,2}, and ECE UYKUR¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf — ²Technische Universität Dresden — ³Renmin University of China — ⁴Universität Stuttgart

In the present study, we use optical pump-probe spectroscopy in reflection geometry to unravel the dynamics of charge carriers in the magnetic kagome metals GdMn₆Sn₆ and TbMn₆Sn₆. The measured pump-probe traces reveal two exponential decay processes and a slow thermal relaxation, similarly to what has been observed in other kagome metals. The exponential decays occur on quite different time scales, and we ascribe them to the dynamics of different types of charge carriers present in the compounds. Additionally, a damped oscillation feature appears during the first 15-20 picoseconds. It can be explained in the context of acoustic strain waves, generated due to a thermal expansion at the sample's surface that is induced by the pump pulse. We also present temperature and pump fluence dependence for both compounds that helps to understand better the relaxation mechanisms.

15 min. break

TT 13.7 Mon 16:45 H 3010

Visualizing many body phases in a partially filled kagome flat band — CAIYUN CHEN, JIANGCHANG ZHENG, YUMAN HE,

RUOPENG YU, SOUMYA SANKAR, KAM TUEN LAW, HOI CHUN PO, and •BERTHOLD JÄCK — HKUST, Department of Physics, Clear Water Bay, Kowloon, Hong Kong SAR, China

The kagome lattice with spin-orbit coupling exhibits a topologically non-trivial flat band in which the effect of Coulomb interactions between the localized charge carriers is believed to be strong. Hence, material realizations of the kagome lattice provide a promising platform to search for new quantum phases of matter at the confluence of topology and strong electronic correlations. We previously showed that the kagome metal CoSn exhibits a quasi-two-dimensional flat band whose occupied electronic states are strongly localised in real space [1].

Here, we study the low energy density of states of $\text{Co}_{1-x}\text{Fe}_x\text{Sn}$ in which partial flat band fillings are realised by hole-doping with Fe. We will present results from temperature-dependent scanning tunnelling microscopy measurements on $\text{Co}_{1-x}\text{Fe}_x\text{Sn}$. Combining high-resolution spectroscopy with spectroscopic imaging on samples with different doping levels x , we observe a rich sequence of states appearing at the Fermi energy that cannot be explained within a single-particle picture. We will discuss our findings in the context of electron-electron interaction induced many body states at partial flat band fillings.

We gratefully acknowledge support by the Hong Kong RGC and the Croucher Foundation.

[1] C. Chen et al., arXiv:2308.08976 (2023)

TT 13.8 Mon 17:00 H 3010

High-pressure infrared spectroscopy study on magnetic kagome metal Fe_3Sn_2 — •ECE UYKUR^{1,2}, MAXIM WENZEL², FRANCESCO CAPITANI³, QI WANG⁴, HECHANG LEI⁴, STEPHAN WINNERL¹, and MARTIN DRESSEL² — ¹Helmholtz-Zentrum Dresden-Rossendorf, Inst. Ion Beam Phys. & Mat. Res., 01328 Dresden, Germany — ²1. Physikalisches Institut, Universität Stuttgart, 70569, Stuttgart, Germany — ³Synchrotron SOLEIL, 91192, Saint-Aubin, France — ⁴Renmin University of China, 100872, Beijing, China

We present a high-pressure broadband optical study of ferromagnetic kagome metal Fe_3Sn_2 at room temperature up to 18 GPa. Different contributions to the optical spectra have been discussed and compared with the DFT calculations, which use the experimental high-pressure crystal structure. Infrared spectra reveal the signatures of conventional and unconventional charge carriers in the compound. While the low-energy spectral range reflects the response of the mobile charge carriers and is significantly modified with increasing pressure, the high energy range shows the modification of the interband transitions in the compound. We also observe the appearance of a sharp plasma edge at energies below 300 cm^{-1} that gradually shifts to the higher energy range in accordance with the appearance of a new Fermi surface under pressure.

TT 13.9 Mon 17:15 H 3010

Broadband optical investigations of the antiferromagnetic kagome metal FeGe — •MAXIM WENZEL¹, ALEXANDER A. TSIRLIN², SUDIP PAL¹, RENJITH MATHEW ROY¹, CHANDRA SHEKHAR³, CLAUDIA FELSER³, ECE UYKUR⁴, ARTEM V. PRONIN¹, and MARTIN DRESSEL¹ — ¹1. Physikalisches Institut, Universität Stuttgart, Germany — ²Felix Bloch Institute for Solid-State Physics, Leipzig University, Germany — ³Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — ⁴Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Germany

Hexagonal FeGe is a two-dimensional kagome metal with the intricate coexistence of magnetism and charge-density-wave (CDW) order. Here, we present a broadband optical spectroscopy study of the antiferromagnetic compound down to 10 K. The contributions of itinerant and localized charge carriers to the optical spectra are comparatively discussed and signatures of the emerging CDW state below approximately 100 K are unveiled. Aided by DFT calculations, we show that

the low-energy interband transitions are very sensitive to small changes of the Fermi level and uncover a delicate interplay between phonons, charge order, and localized carriers.

TT 13.10 Mon 17:30 H 3010

Unveiling a Kagome Metal Candidate with m-type Van Hove Singularity at Fermi Level: Theoretical Exploration and Electronic Features — •ANJA WENGER — University of Würzburg, Germany

We embark on theoretically identifying universality classes of promising kagome metal candidate materials still to be realized in experiment. We intend to reach an electronic correlation strength still ensuring electronic itineracy. Conducting a free energy analysis of our proposed material candidate as a function of volume reveals a minimum at unstrained volume. This holds true even for the structural distortions exhibited by the material, i.e., a twisted and breathing kagome configuration. Remarkably, we generically obtain a mixed-type van Hove singularity in close proximity to the Fermi level. The results were obtained employing both, ab-initio calculations in the framework given by density functional theory (DFT), and crystal field analysis. Our proposed kagome material promises to exhibit exotic electronic features, opening new possibilities for exploring unprecedented quantum phenomena in kagome metals.

TT 13.11 Mon 17:45 H 3010

Spin-orbit coupling effects in a kagome scattering network — •PATRIK WITTIG¹, FERNANDO DOMINGUEZ¹, and PATRIK RECHER^{1,2} — ¹Institute of Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — ²Laboratory of Emerging Nanometrology, 38106 Braunschweig, Germany

Recently, scattering networks have gained a lot of attention, because they can model two-dimensional Dirac systems that are dominated by valley chiral modes. Here, we study the kagome scattering network that has been proposed in double-aligned graphene-hexagonal boron nitride [1,3] and periodically strained graphene [2]. By combining scattering matrices, we transform the kagome network to a triangular network with an energy-dependent scattering matrix and perform magnetotransport calculations. Additionally, due to the recent interest in proximity-induced spin-orbit effects in graphene, we include spin-orbit coupling in the scattering network model.

[1] C. Mouldale et al., Phys. Rev. B 105 (2022) L201112.

[2] C. De Beule et al., Phys. Rev. B 107(2023) 045405.

[3] F. K. de Vries et al., arXiv: 2303.06403.

TT 13.12 Mon 18:00 H 3010

Magnetocrystalline and charge transport anisotropy in metallic Kagome ferromagnet Fe_3Sn — •LILIAN PRODAN¹, VLADIMIR TSURKAN^{1,2}, and ISTVAN KEZSMARKI¹ — ¹Experimentalphysik V, Institute of Physics, Augsburg University, D-86159 Augsburg, Germany — ²Institute of Applied Physics, Moldova State University, MD 2028, Chisinau, R. Moldova

Electron correlated Kagome magnets have recently been recognized as a versatile platform to investigate the interplay between the topology of the electronic band structure, magnetism and emergent novel topological states. Topological band effects were also invoked for explanation of the giant 'anomalous' anisotropy of the longitudinal conductivity and off-diagonal Hall resistivity. Here we report the interplay of magnetocrystalline anisotropy (MAE) and charge transport in metallic Kagome ferromagnet Fe_3Sn . We revealed an 'anomalous' anisotropy of the longitudinal resistivity and anomalous Hall resistivity (AAHR). The linear scaling of AAHR with the MAE suggests that the anisotropic charge transport in Fe_3Sn is governed by the strong spin-orbit coupling. Our results provide new insight into elucidation of interplay of crystal structure, charge transport and magnetism in the iron-based Kagome metallic magnets.