TT 23: Kagome Systems

Time: Tuesday 9:30-13:00

TT 23.1 Tue 9:30 HSZ 304 Broadband optical investigations of the CDW state in Kagome metals AV_3Sb_5 (A = K, Rb, Cs) — •E. UYKUR^{1,2}, M. WENZEL¹, B.R. ORTIZ^{3,4}, S.D. WILSON⁴, S. WINNERL², M. DRESSEL¹, and A. A. TSIRLIN⁵ — ¹1. Physikalisches Institut, Universität Stuttgart, 70569, Stuttgart, Germany — ²Helmholtz-Zentrum Dresden-Rossendorf, Inst. Ion Beam Phys. & Mat. Res., 01328 Dresden, Germany — ³Materials Department and California Nanosystems Institute,University of California Santa Barbara, Santa Barbara, CA, 93106, United States — ⁴Materials Department, University of California Santa Barbara, Santa Barbara, CA, 93106, United States — ⁵Felix Bloch Institute for Solid-State Physics, Leipzig University, 04103 Leipzig, Germany

We present a broadband optical study of non-magnetic Kagome metals AV_3Sb_5 (A = K, Rb, Cs) down to 10 K. Different contributions to the optical spectra have been discussed and compared with the DFT calculations in normal and charge density wave (CDW) states. Spectra reflect the response of the 2D Dirac fermions and are frequencyindependent in a broad energy range. Low energies are governed by the itinerant and localized charge carriers that show a spectral weight redistribution below the CDW transition. Our results show that the CDW gaps evolve systematically between the siblings (K<Cs<Rb) in line with their transition temperatures. We further use the experimental spectral weight to gauge the effect of electronic correlations and find it increasing with reducing the size of A.

TT 23.2 Tue 9:45 HSZ 304

Complex charge order in the AV_3Sb_5 kagome metals — •MORTEN CHRISTENSEN¹, TURAN BIROL², BRIAN ANDERSEN¹, and RAFAEL FERNANDES³ — ¹Niels Bohr Institute, University of Copenhagen — ²Department of Chemical Engineering and Materials Science, University of Minnesota — ³School of Physics and Astronomy, University of Minnesota

The kagome lattice, consisting of an array of corner-sharing triangles, offers a rich platform to study the behavior of correlated electrons. In kagome metals, the electronic band structure exhibits Dirac points, flat bands, and van Hove singularities - features which promote the role of electronic correlations. A family of recently discovered kagome metals, AV_3Sb_5 (A=K, Rb, Cs), provides a realization of these features. These materials exhibit an enigmatic superconducting order, which emerges from a three-dimensional charge-density wave (CDW) phase. While the precise nature of the CDW phase is still unknown, there are indications of both time-reversal symmetry breaking and nematicity inside the charge-ordered phase. Starting from from the low-energy electronic states near the van Hove singularities, we construct a phenomenological model to describe the CDW phase. The order parameters of this model are either real, corresponding to bond distortions, or imaginary, corresponding to loop-currents. These CDW orders can coexist or compete which results in a rich landscape of subsidiary orders, including various types of multipolar magnetic orders. These have unique experimental signatures which can aid in pinpointing the precise nature of the CDW phase observed in experiments.

TT 23.3 Tue 10:00 HSZ 304

Investigation of the charge density wave in single crystal CsV_3Sb_5 under hydrostatic pressure — •FABIAN STIER¹, TO-BIAS RITSCHEL¹, MAREIN RAHN¹, CHANDRA SHEKHAR², CLAUDIA FELSER², and JOCHEN GECK¹ — ¹IFMP, TU Dresden, Germany — ²MPI CPfS, Dresden, Germany

The topological Z_2 kagome materials AV₃Sb₅ (A = K, Rb, Cs) show a nontrivial electronic topology, exhibit superconductivity (SC) and a charge-density-wave (CDW) order. CsV₃Sb₅ shows a CDW below 90K with a 2x2x4 superstructure, which changes around 60K to a 2x2x2 superstructure. To investigate the interplay of CDW-order and SC we performed single crystal x-ray diffraction under hydrostatic pressure, with Argon as a pressure medium, up to 2 GPa and 20K. In this pressure range the SC shows two distinct domes, where Tc is enhanced and shows two maxima. The 2x2x2 CDW at low temperatues persists under pressure range both, the CDW and a new emerging incommensurate CDW coexists. While the first CDW quickly vanishes, the incommensurate CDW persists up to pressures where the SC shows

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another extremum in T_c. Above this pressure, \sim 1.5GPa, no CDW could be detected. An accurate knowledge of these structural modifications will be essential to explain the relationship of topology and superconductivity in this class of materials.

TT 23.4 Tue 10:15 HSZ 304 Indication of a strong coupling charge density wave in CsV_3Sb_5 — •LEANDER PEIS^{1,2,3}, GE HE^{1,4}, and RUDOLF HACKL^{1,2,3} — ¹Walther Meissner Institut, Bayerische Akademie der Wissenschaften, Garching 85748, Germany — ²Technische Universität München, Garching 85748, Germany — ³IFW Dresden, Dresden 01062, Germany — ⁴University College Cork, Cork, Ireland

A prominent example for studying the interplay of electronic correlations and non-trivial topology is the material class of AV_3Sb_5 (A=K,Rb,Cs), displaying unconventional charge order in the range of 100 K and superconductivity at temperatures below 2.5 K. Here, we present a polarization-dependent Raman scattering study of the Kagome metal CsV₃Sb₅, focusing on the charge density wave (CDW). We resolve several signatures of strong-coupling between the lattice and the electronic system. First, the energy of the A_{1a} Γ -point phonon exhibits a discontinuity at the phase transition temperature $T_{CDW} = 95 \,\mathrm{K}$. Second, the magnitude and symmetry dependence of the observed CDW energy gap 2Δ suggest strong coupling and a substantial anisotropy. Third, the observed A_{1g} amplitude mode depends weaker on temperature than expected and displays an asymmetric Fano-type line shape, particularly around 70 K. We interpret this deviation in terms of strong coupling between the phonon-like amplitude mode and the electronic continuum. To the best of our knowledge such an asymmetry of an amplitude mode has not been observed before.

TT 23.5 Tue 10:30 HSZ 304

X-ray diffraction on the charge-density wave in the Kagome superconductor RbV_3Sb_5 — •SABREEN HAMMOUDA¹, YU-HUI LIANG², PO-CHUN CHANG², CARSTEN PAULMANN³, YISHUI ZHOU¹, ADRIAN MERRIT¹, PIKESH PAL¹, RAHAF YASEEN¹, HONGXIONG LIU⁴, YOUGUO SHI⁴, CHAO-HUNG DU², and YIXI SU¹ — ¹JCNS-MLZ, Forschungszentrum Jülich, 85748 Garching, Germany — ²Dept. of Phys., Tamkang University, Tamsui 251, Taiwan — ³DESY, 22607 Hamburg, Germany — ⁴IOP, CAS, Beijing 100190, China

The newly discovered Kagome superconductors AV₃Sb₅ (A=K, Rb or Cs), in which non-trivial band topology, charge-density wave (CDW), and superconductivity are intertwined, have attracted tremendous interests. Despite extensive recent investigations via X-ray diffraction (XRD) and other complementary local probe techniques, it remains a major challenge to gain a consistent picture of the CDW modulation across different AV₃Sb₅ samples. In this talk, we will present our recent single-crystal XRD investigations (in-house and synchrotron) of the CDW modulations over a wide temperature range in the lessstudied RbV₃Sb₅. A unique CDW modulation of the 2x2x2 type can be confirmed for RbV_3Sb_5 below $T_{CDW} = 102$ K, and no evidence for CDW fluctuations above T_{CDW} could be found. Our detailed temperature dependence measurements of the CDW superstructure reflections indicate a second-order phase transition with a 2D Ising character. A comparison to other AV₃Sb₅ compounds and possible implications on the understanding of the nature of the CDW in these Kagome superconductors will be given.

TT 23.6 Tue 10:45 HSZ 304 \mathbb{Z}_2 topological insulator and Hubbard interactions on the Kagome lattice — IRAKLI TITVINIDZE¹, •JULIAN LEGENDRE^{2,3}, MAARTEN GROTHUS¹, BERNHARD IRSIGLER¹, KARYN LE HUR², and WALTER HOFSTETTER¹ — ¹Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany — ²CPHT, CNRS, Institut Polytechnique de Paris, Route de Saclay, 91128 Palaiseau, France — ³Department of Physics and Materials Science, University of Luxembourg, 1511 Luxembourg, Luxembourg

The study of topological phase transitions has been a very active field of research since the 80's; in recent decades topological insulators have been one of the major foci in this field. Understanding the role of the interactions in such systems is also currently is major challenge for the scientific community. In this talk, I will present a study of a time-reversal invariant topological model, with Hubbard interactions, on the Kagome lattice. The topological model contains intrinsic and Rashba spin-orbit coupling terms and position-dependent onsite energies. Relying on several analytical methods, I will show how the \mathbb{Z}_2 topological phase, resulting from the flux term, is tuned by varying the amplitude(s) of on-site energy terms and/or of the Rashba spin-orbit coupling term, at filling n = 2/3. Then, we will study the effect of Hubbard interactions on the topological properties for a specific on-site energy configuration and at vanishing Rashba spin-orbit coupling. We will use perturbation theory in the large Hubbard amplitude U limit and a mean-field method for smaller U. I will compare these analytical results with numerical results obtained by our collaborators.

TT 23.7 Tue 11:00 HSZ 304

Temperature-dependent pump-probe spectroscopy of the magetic Kagome metal $Fe_3Sn_2 - \bullet M$. G. FARIA¹, Q. WANG², H. C. LEI², A. PASHKIN¹, S. WINNERL¹, M. HELM^{1,3}, and E. UYKUR¹ - ¹Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany - ²Department of Physics and Beijing Key Laboratory of Opto-electronic Functional Materials & Micro-nano Devices, Renmin University of China, 100872 Beijing, China - ³Institute for Applied Physics, Technische Universität Dresden, 01069 Dresden, Germany

In this study, we present optical pump-probe measurements on a magnetic Kagome metal, Fe_3Sn_2 , under different temperatures down to 10 K. The obtained spectra can be fitted with a double exponential decay, indicating that the system has two distinct relaxation processes. Additionally, some unexpected and pronounced oscillations are dominating the spectra, giving evidence of a strong electron-phonon coupling in Fe_3Sn_2 , at least in this ultra-fast regime. The frequency of this coupled phonon is determined to be around 2.5 THz. Finally, we will discuss the temperature and pump fluence dependence of the observed phonon coupling and the distinct relaxation dynamics in this material.

15 min. break

TT 23.8 Tue 11:30 HSZ 304

Complex magnetic orders and the emergent topological Hall effect in the kagome metal ErMn_6Sn_6 — •YISHUI ZHOU¹, CHANGJIANG YI², DMITRY KHALYAVIN³, FABIO ORLANDI³, PASCAL MANUEL³, SABREEN HAMMOUDA¹, ADRIAN MERRITT¹, CLAUDIA FELSER², THOMAS BRÜCKEL⁴, and YIXI SU¹ — ¹JCNS-MLZ, Forschungszentrum Jülich GmbH, Garching, Germany — ²Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — ³ISIS Neutron & Muon Facility, STFC, Rutherford Appleton Laboratory, Didcot, UK — ⁴JCNS-2 & PGI-4, Forschungszentrum Jülich GmbH, Jülich, Germany

Following the discovery of a quantum-limit magnetic Chern phase in $TbMn_6Sn_6$, the magnetic topological metal series RMn_6Sn_6 (R=Gd-Yb, and Y, Lu, etc.), that possesses an ideal Kagome lattice of Mn, has emerged as a new platform to explore exotic states and novel functionalities. We have recently carried out the growth of high-quality single crystals of the magnetic Kagome metal $ErMn_6Sn_6$, and the physical properties characterizations via the magnetic susceptibility, heat capacity, and Hall conductivity measurements. We have also undertaken comprehensive neutron diffraction experiments on both single-crystal and powder samples at the WISH diffractometer at ISIS. Our study has clearly hinted a fascinating interplay between topologically non-trivial electronic band structures, magnetism and electronic correlations in $ErMn_6Sn_6$.

TT 23.9 Tue 11:45 HSZ 304

Thermodynamics of the spin-half square Kagome lattice antiferromagnet — •JÜRGEN SCHNACK¹, OLEG DERZHKO², and JO-HANNES RICHTER³ — ¹Fakultät für Physik, Universität Bielefeld, D-33501 Bielefeld, Germany — ²Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 79011 Lviv, Ukraine — ³Institut für Physik, Universität Magdeburg, D-39016 Magdeburg & Max-Planck-Institut für Physik Komplexer Systeme, D-01187 Dresden, Germany

Over the last decade, the interest in the spin-1/2 Heisenberg antiferromagnet (HAF) on the square Kagome lattice has been growing as a model system of quantum magnetism with a quantum paramagnetic ground state, flat-band physics near the saturation field, and quantum scars. Here, we present large-scale numerical investigations of the specific heat, the entropy, as well as the susceptibility by means of the finite-temperature Lanczos method for system sizes of N = 18, ..., 54. We find that the specific heat exhibits a low-temperature shoulder below the major maximum which can be attributed to low-lying singlet excitations filling the singlet-triplet gap, which is significantly larger than the singlet-singlet gap. For the susceptibility the singlet-triplet gap leads to an exponentially activated low-temperature behavior. The maximum of the susceptibility is found at a pretty low temperature T/J = 0.146 (for N = 42). We find a striking similarity of our data with the corresponding ones for the Kagome HAF down to very low temperatures.

TT 23.10 Tue 12:00 HSZ 304

Asymmetric melting of the 1/3-plateau for the Kagome lattice antiferromagnet — •HENRIK SCHLÜTER¹, JÜRGEN SCHNACK¹, and JOHANNES RICHTER² — ¹Bielefeld University, Bielefeld, Germany — ²University of Magdeburg and MPIPKS Dresden, Germany

The Kagome lattice Heisenberg antiferromagnet (KHAF) is a rich source of unconventional physics not only regarding its spin-liquid ground state but also with respect to its behavior at non-zero field and temperature.

Here we investigate the phenomenon of the asymmetric melting of the magnetization plateau at 1/3 of the saturation magnetization, see Refs.[1, 2]. We explain the effect by discussing the energy diagram and the density of states constructed from finite-temperature Lanczos data for KHAF with up to 48 sites [3].

 J. Schnack, J. Schulenburg, J. Richter, Phys. Rev. B 98, 094423 (2018)

[2] Takahiro Misawa, Yuichi Motoyama, and Youhei Yamaji, Phys. Rev. B 102, 094419 (2020)

[3] H. Schlüter, F. Gayk, H.-J. Schmidt, A. Honecker, J. Schnack, Z. Naturforsch. A 76, 823 (2021)

TT 23.11 Tue 12:15 HSZ 304

Classical and quantum frustrated models of planar X-Y spins on the Kagome lattice: anisotropic magnetic patterns — •OLIVER NEYENHUYS, MIKHAIL FISTUL, and ILYA EREMIN — Ruhr Universität Bochum

We present a theoretical study of various highly anisotropic magnetic patterns occurring in the geometrically frustrated model of planar X-Y spins on the Kagome two-dimensional lattice. Frustration is introduced by a specific spatial arrangement of both ferromagnetic and anti-ferromagnetic bonds between adjacent magnetic moments on the lattice vertices. At the critical value of frustration f = 3/4 such a system displays the phase transition from an ordered ferromagnetic state to frustrated regime featuring a highly degenerate ground state in which topological (anti)vortices penetrate each cell. Taking into account a generous amount of topological constraints, the thermal fluctuations and the quantum tunneling induced transitions between these vortices/anti-vortices, we derive an effective Ising spin Hamiltonian on the corresponding hexagonal lattice, in which a strong long-range interaction between a well separated (anti)vortices occurs. By making use of the mean field analysis and direct numerical diagonalization of the Hamiltonian we characterize various classical and quantum phases and phase transitions between them for large and small Kagome lattices. Experimental observation of such magnetic patterns with coherent networks of superconducting qubits will be discussed.

TT 23.12 Tue 12:30 HSZ 304 Magnon-phonon coupling in the Kagome-lattice antiferromagnet Mn_3Ge — •Aleksandr Sukhanov, Nikita Andriushin, Anton Kulbakov, and Dmytro Inosov — Institut für Festkörperund Materialphysik, Technische Universität Dresden, D-01069 Dresden Magnons and phonons, which are quanta of spin excitations and crystal-lattice vibrations in ordered materials, respectively, can be strongly coupled together when their dispersion relations intersect in reciprocal space. This results in hybridised collective spin-lattice excitations, also known as magnetoelastic (ME) modes.

The metallic hexagonal compound Mn_3Ge is characterized by a noncollinear spin order due to the geometric frustration of the Kagome lattice formed by Mn ions. Our earlier studies showed that Mn_3Ge belongs to a rare class of materials that possess very strong ME coupling. The ME effect is manifested in the large negative thermal expansion of the material and high-pressure tuning of its remarkable anomalous Hall effect. Most intriguing is a previous observation that the noncollinear spin structure of Mn_3Ge can be driven into a collinear ferromagnetic state under a hydrostatic pressure of ~5 GPa. This, in turn, provides hints on how the magnetic structure is linked to the unconventional electron transport phenomena in this material.

In this talk, we will discuss the results of our recent single-crystal

inelastic neutron and x-ray scattering spectroscopy measurements of Mn_3Ge . We were able to clearly resolve momenta and energy of the ME hybridization. The experimental results are supported with the first-principle lattice dynamics calculations.

TT 23.13 Tue 12:45 HSZ 304

Raman scattering study of magnetism in the Kagome materials Fe_3Sn_2 and $Co_3Sn_2S_2 - \bullet$ RUDI HACKL^{1,2,3}, GE HE⁴, and LE-ANDER PEIS^{1,2,3} - ¹Walther-Meissner-Institut, 85748 Garching, Germany - ²Technische Universität München, 85748 Garching, Germany - ³IFW Dresden, Dresden 01062, Germany - ⁴University College Cork, Cork, Ireland

 $\rm Fe_3Sn_2$ and $\rm Co_3Sn_2S_2$ have triangularly coordinated layers of 3d transition metal ions sitting on a Kagome network. Both compounds have Dirac and Weyl nodes in the band structure. $\rm Fe_3Sn_2$ is ferromagnetic

below 670 K, and the spins start to reorient from perpendicular to parallel to the Kagome layer below 150 K. This reorientation was first observed by Mössbauer spectroscopy but has in general little influence on other observables such as thermal expansion or magnetization. In our Raman study we find an anomaly of the line width and the energy of the lowest A_{1g} phonon where the Sn atoms vibrate perpendicular to the Fe plane. We interpret the anomaly in terms of an enhanced spin-phonon coupling below approximately 150 K. $Co_3Sn_2S_2$ starts ordering antiferromagnetically below 175 K and turns into a ferromagnet in the low-temperature limit. Here, the spins are first in plane and the order is nearly frustrated. Below 100 K the spins point along the *c*-axis and are parallel. The A_{1g} phonon couples strongly to a continuum as highlighted by the asymmetric Fano-type line shape. The asymmetry is maximal close to the magnetic transition. We argue that small changes of the lattice have an effect on the magnetism.