TT 10: Correlated Electrons: Other Materials

Time: Monday 15:00–18:15 Location: HSZ 204

TT 10.1 Mon 15:00 HSZ 204

Towards a complete quantum oscillatory assessment of the Fermi surface of CoSi — •Nico Huber[1], Simon Röder[1], Georg Benka[1], Andreas Bauer[1], Sanu Mishra[2,3], Ilya Sheikin[2], Christian Pfleiderer[1], and Marc A. Wilde[1] — [1]Physik-Department, TU Munich, D-85748 Garching, Germany — [2]LNCMI-CNRS, Grenoble, France — [3]Los Alamos National Laboratory, Los Alamos, USA

The B20 compound CoSi has recently attracted great interest due to its electronic structure hosting multifold fermions at the Γ- and R-point [1] and topologically non-trivial nodal planes on the Brillouin zone boundary [2,3]. While quantum oscillations (QOs) arising from the Fermi surface (FS) around the R-point have been studied in great detail and are well understood [3,4], only limited information has been presented on QOs related to the FS around the Γ-point [5]. Here, we report the experimental identification of previously unobserved QOs arising from heavy FS sheets around Γ in the Shubnikov-de Haas and de Haas-van Alphen spectra of CoSi. The oscillation frequencies, their angular dispersion, and the associated effective masses are in good agreement with first principle calculations. Our observations confirm the calculated bandstructure of CoSi, thus completing the experimental verification of the Fermi surface based on quantum oscillations.

[1] Rao *et al.*, Nature **567**, 496 (2019)
Sanchez *et al.*, Nature **567**, 500 (2019)
[2] Wilde *et al.*, Nature **594**, 374 (2021)
[3] Huber *et al.*, PRL **129**, 026401 (2022)
[4] Guo *et al.*, Nat. Phys. **18**, 813 (2022)
[5] Wang *et al.*, PRB **102**, 115129 (2020)
Sasmal *et al.*, J. Phys.: Condens. Matter **34**, 425702 (2022)

TT 10.2 Mon 15:15 HSZ 204

Miniaturized setup for quantum oscillatory studies under temperature modulation — •Michelle Hollricher, Christian Pfleiderer, and Marc A. Wilde — Physik-Department, Technical University of Munich, D-85748 Garching, Germany

Measurements of the magnetization and its derivatives provide fundamental insights into the magnetic properties of metals. In particular this is true for magnetic quantum oscillations. We report the development of a miniaturized setup for direct measurements of the temperature derivative of the magnetization as a function of magnetic field and temperature, using a modular setup comprising AC heating with inductive signal pick-up. The dimensions of our setup have been optimized to permit use in combination with standard mechanical rotators, this way enabling measurements of the magnetization as a function of magnetic field orientation down to ultra-low temperatures. Following thorough characterization of the frequency response of our miniaturized setup, we revisited the de Haas-van Alphen effect in bismuth, focusing on the electronic structure of the electron pockets.

TT 10.3 Mon 15:30 HSZ 204

Torque magnetometry of FeSi at low temperatures — •Carolina Burger, Vivek Kumar, Andreas Bauer, and Christian Pfleiderer — Physik-Departement, Technical University of Munich, D-85748 Garching, Germany

We report a study of the torque magnetization of the correlated small-band-gap semiconductor FeSi in the regime of the saturation of the resistivity at temperatures below a few Kelvin. The magnetic field dependence of the electrical transport properties provides strong circumstantial evidence of a high-mobility surface conduction channel, that is insensitive to the additional presence of an impurity band in the bulk [1, 2]. The surface conduction channel shares great similarities with properties reported for topological insulators, but displays a striking lack of sensitivity to the presence of ferromagnetic impurities as studied by means of a series of single crystals with slightly different starting compositions. We discuss the torque magnetization observed in FeSi with respect to key characteristics observed in the field-polarized state of isostructural magnetic B20 compounds such as MnSi or $Fe_{1-x}Co_xSi$.

[1] Y. Fang, et al., Proc. Natl. Acad. Sci. 115, 8558 (2018)
[2] B. Yang, et al., Proc. Natl. Acad. Sci. 118, e2021203118 (2021)

TT 10.4 Mon 15:45 HSZ 204

Metal-insulator transition and onset of magnetic order in $Fe_{1-x}Co_xSi$ — •Julius Grefe[1], Philipp Herre[1], Yannis Hilgers[1], Felix Labbus[1], Nina Lüer[1], Mauricio de Melo[1,2], Jochen Litterst[1], Stefan Süllow[1], and Dirk Menzel[1] — [1]Inst. für Physik der Kondensierten Materie, Technische Universität Braunschweig, Germany — [2]Departamento de Fisica, Universidade Estadual de Maringá, Brazil

The B20 transition metal silicides (Fe,Co,Mn)Si have been under investigation for many decades. Although the general observations regarding the electronic and magnetic properties are similar, various details of the phase diagram of $Fe_{1-x}Co_xSi$ are not yet well-established. We have prepared a series of $Fe_{1-x}Co_xSi$ single crystals and investigated the metal-insulator transition as well as the onset of magnetic order in the low Co percentage range by means of transport and susceptibility measurements. In addition, we present for the first time single-crystal Mössbauer spectroscopy experiments in order to complement our study using a microscopic probe. Our investigation sheds light on the physics of quantum criticality and metal-insulator transition and their interplay in the regime of small Co concentrations.

TT 10.5 Mon 16:00 HSZ 204

Temperatur dependence of the lattice constants of $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$ — •Tobias Konrad, Alexander Engelhardt, Christoph Resch, Andreas Bauer, and Christian Pfleiderer — Physik Department, Technical University Munich, D-85748 Garching, Germany

When magnetic order in the chiral magnet MnSi is suppressed under hydrostatic pressure, topological non-Fermi-liquid behavior emerges, where neutron Larmor diffraction of the lattice constants establishes the absence of quantum criticality [1-3]. Magnetic order in MnSi may also be suppressed by substitutional replacement of iron or cobalt on the manganese sites [4,5]. Using powder x-ray diffraction, we have studied the temperature dependence of the lattice constants of $Mn_{1-x}Fe_xSi$ ($0 \leq x \leq 0.22$) and $Mn_{1-x}Co_xSi$ ($0 \leq x \leq 0.04$) between room temperature and $\sim 12\,K$. The evolution of the lattice constants as a function of iron and cobalt concentration is discussed in comparison to changes of the lattice constants of MnSi under hydrostatic pressure.

[1] C. Pfleiderer et al., Nature **414**, 427 (2001)
[2] C. Pfleiderer et al., Science **316**, 1871 (2007)
[3] R. Ritz et al., Nature **497**, 231 (2013)
[4] A. Bauer et al., Phys. Rev. B **82**, 064404 (2010)
[5] J. Kindervater et al., Phys. Rev. B **101**, 104406 (2020)

TT 10.6 Mon 16:15 HSZ 204

Effect of anion substitution on the Mott insulating instability in the organic conductors κ-(BEDT-TTF)$_2$X studied 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

The layered organic charge-transfer salts κ-(BEDT-TTF)$_2$X have been extensively employed as model systems for studying the Mott metal-insulator transition. The insulating instability in these materials is very sensitive to external pressure and to minor chemical changes, e.g., variation of the insulating anion. The anion substitution is broadly believed to act similarly to pressure, leading to a modification of the correlation strength ratio U/t. However, recent first-principles band-structure calculations [1] suggest that anion substitution in κ salts influences the ground state chiefly through the spin-frustration effect by changing the transfer-integral anisotropy ratio t'/t rather than through U/t. Here we report on comparative studies of magnetic quantum oscillations in the salts with X = NCS, Cl, and Br, aiming at disentangling the roles of the electronic correlations and spin frustration in the insulating instability within this family.

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

15 min. break

TT 10.7 Mon 16:45 HSZ 204

Mott criticality in the deuterated variant of κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br studied by thermal expansion under He-gas pressure — •Yassine Agarmani, Harald Schubert, Bernd Wolf, and Michael Lang — PI, GU Frankfurt, CRC/TRR288, DE

The understanding of the nature of the critical behavior at the Mott transition has recently been given a new twist by thermodynamic measurements on the Mott insulator κ-(ET)$_2$Cu[N(CN)$_2$]Cl (κ-Cl)]. While so far mainly electronic scenarios have been considered to describe the Mott transition, the observations of strong non-linearities in the strain-stress relation around the Mott critical endpoint in κ-Cl showed that the lattice degrees of freedomn play a crucial role [1]. This behavior has been found to be consistent with the proposed scenario of critical elasticity [2], which considers a non-perturbatively strong coupling of the elastic- to the electronic degrees of freedom, causing a softening of the lattice. These observations raise the question of the implication of critical elasticity for our understanding of the general phase diagram of the κ-(ET)$_2$X family. To address this question, we have chosen a system related to κ-Cl, namely the fully deuterated κ-(ET)$_2$Cu[N(CN)$_2$]Br, which is known to be near the Mott critical endpoint at ambient pressure. By using an extension [3] of the setup used in [1], which enables us to fine-tune the He-gas pressure while performing high-resolution measurements of length changes, we aim to compare our results with those on κ-Cl in terms of the extension of the range of critical elasticity.

[1] Gati et al., Sci. Adv. 2, e1601646 (2016)
[2] Zacharias et al., PRL 109, 176401 (2012)
[3] Agarmani et al., RSI 93, 113902 (2022)

TT 10.8 Mon 17:00 HSZ 204

Effect of uniaxial strain on the phononic and electronic excitations of Ta_2NiS_5 — •Mai Ye, Amir-Abbas Haghighirad, and Le Tacon Matthieu — Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany

Semiconductor Ta_2NiS_5 exhibits a structural transition from orthorhombic phase to monoclinic phase at 120 K, driven by acoustic instability [1]. Two Raman-active phonon modes, which have the same symmetry as the order parameter (B_{2g} symmetry), show continuous frequency softening on cooling from 300 K to 20 K. Moreover, a sharp exciton mode in the B_{2g} symmetry channel has been observed at 0.3 eV. We study the phonon modes and interband excitations of Ta_2NiS_5 under uniaxial strain at low temperature. With increasing tensive strain along crystallographic a axis, the frequency of the two B_{2g}-symmetry phonon modes and the band gap of this semiconductor both increase, with a 6.5% frequency increase of the lowest-energy B_{2g} phonon mode corresponding to a 4.1% increase of the gap size. On the contrary, the frequency change of the non-softening phonons is less than 1%. By analyzing the phonon intensity, we further find that the magnitude of the order parameter, and in turn the phase transition temperature, increases with the tensive strain. These experimental results demonstrate Ta_2NiS_5 as a suitable platform to explore the manipulation of lattice dynamics and electronic structure by applying uniaxial strain.

[1] Phys. Rev. B 104, 045102 (2021)

TT 10.9 Mon 17:15 HSZ 204

Magnetic anisotropy and low-energy spin dynamics in magnetic van der Waals compounds $Mn_2P_2S_6$ and $MnNiP_2S_6$ — •Joyal John Abraham[1,2], Yurii Senyk[1], Yuliia Shemerliuk[1], Sebastian Selter[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

We report a comprehesive high-field electron spin resonance (ESR) study performed on single crystals of $Mn_2P_2S_6$ and $MnNiP_2S_6$ in the broad ranges of temperatures, frequencies and magnetic fields. Analysing the antiferromagnetic modes well below the ordering temperature T_N, we have found that the ground state, the order type and magnetic anisotropy (MA) change with increasing x in $(Mn_{1-x}Ni_x)_2P_2S_6$. In the case of $Mn_2P_2S_6$, an application of the linear spin wave theory enabled us to determine the anisotropy and exchange constants, important for a quantitative description of the ground state. A systematic increase of the g-factor and its anisotropy, measured at $T \gg T_N$, is observed with increasing Ni content, which, in turn, sheds light on the nature of MA in the ordered state. The investigation of the T-dependence of line shifts from the paramagnetic resonance position reveals already well above T_N the presence of the short range spin-spin correlations static on ESR time scale, which are more pronounced in $MnNiP_2S_6$.

TT 10.10 Mon 17:30 HSZ 204

Switching of magnetic anisotropy from out-of-plane to in-plane in quasi-2D van der Waals $(Mn_{1-x}Ni_x)_2P_2S_6$ single crystals — •Yuliia Shemerliuk, Anja U. B. Wolter, Bernd Büchner, and Saicharan Aswartham — Institut für Festkörperforschung, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

In the recent years magnetic two-dimensional van der Waals materials are at the forefront of the research. Magnetism has been extensively investigated in the family of $TM_2P_2S_6$ (TM= Ni, Co, Fe, Mn & V). Transition metal TM substitution has been used as a technique to control magnetism in this family of compounds [1-3]. In this talk, we will present crystal growth by chemical vapor transport together with a thorough structural and magnetic characterization of the quasi-2D magnets $(Mn_{1-x}Ni_x)_2P_2S_6$ with x = 0, 0.3, 0.5, 0.7 & 1. As-grown crystals exhibit a layered morphology with weak van der Waals interlayer interactions parallel to the crystallographic ab plane of the monoclinic symmetry in the space group C2/m (No. 12). In this series, the two neighboring members $Mn_2P_2S_6$ and $Ni_2P_2S_6$ differ in magnetic atoms, magnetic easy axes, spin anisotropy, and nearest neighbor magnetic interactions. The magnetization measurements show an antiferromagnetic ground state for all grown crystals. The magnetic ordering temperature TN shows nonmonotonic behavior. The magnetic anisotropy switches from out-of-plane to in-plane as a function of composition.

TT 10.11 Mon 17:45 HSZ 204

Single crystal growth, structural and transport properties of the Mott insulator $BaCoS_2$ — •Haneen Abushammala, Teslin Thomas, Andreas Kreyssig, and Anna Böhmer — Institute for Experimentalphysik IV, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany.

The quasi-2D $BaCoS_2$ is a Mott insulator with a stripe-like antiferromagnetic ordering at T_N=290 K. Both chemical doping or hydrostatic pressure drive the system into a paramagnetic metallic phase. Interestingly, there is no structural transition at the metal-insulator transition of this phase, which offers ideal conditions to investigate the Mott transition in a model multiband system [1].

Nevertheless, $BaCoS_2$ remains little studied, and the interplay of electronic and structural features is still unclear. High-quality single crystals are needed to elucidate this issue. The synthesis of single-crystalline $BaCoS_2$ is challenging owing to its metastability, with a decomposition into Ba_2CoS_3, CoS and S below 850°C. The $BaCoS_2$ phase can only be obtained via quenching from high temperature. Moreover, $BaCoS_2$ melts incongruently, which calls for a flux growth method necessitating separation of the crystals from the flux by the end of the growth. We have successfully grown single crystals of pure and the hole-doped $BaCoS_2$ using a self-flux method with high-temperature flux separation and quench. The structural and anisotropic electrical transport properties are determined and discussed.

[1] H. Abushammala, B. Lenz, B. Baptiste, M. Casula, Y. Klein and A. Gauzzi, in preparation (2022).

TT 10.12 Mon 18:00 HSZ 204

Spin-orbit entangled crystal-field excitations in $5d^4$ $j = 0$ osmates — •Philipp Warzanowski[1], Marco Magnaterra[1], Philipp Stein[1], Quentin Faure[2], Christoph Sahle[2], Holger Schwab[1], Thomas Lorenz[1], Petra Becker[3], Ladislav Bohatý[3], Paul H. M. van Loosdrecht[1], and Markus Grüninger[1] — [1]Institute of Physics II, University of Cologne — [2]European Synchrotron Radiation Facility, Grenoble Cedex, France — [3]Sect. Crystallography, Institute of Geology and Mineralogy, University of Cologne

For strong spin-orbit coupling, the d^4 electron configuration may show a non-magnetic $j = 0$ ground state. In $5d^4$ iridates, magnetic behavior has been discussed controversially and finally it has been attributed to defects, while excitonic magnetism has been proposed for $4d^4$ ruthenates. We show that the $j = 0$ state is very well realized in the cubic antifluorite-type $5d^4$ osmates K_2OsCl_6 and K_2OsBr_6. The magnetic susceptibility exhibits van-Vleck type magnetism without a sizeable Curie-Weiss contribution. Employing resonant inelastic x-ray scattering (RIXS) and infrared spectroscopy as complementary techniques, we investigate the electronic excitations and determine the electronic parameters by comparison with local multiplet calculations. The cubic crystal-field splitting 10 Dq and the charge transfer energy are 15%

smaller for the chlorine compound than for its bromide sister, whereas the intra-t_{2g} excitation energies are reduced by 4%. This allows us to quantify the influence of the e_g orbitals on the effective spin-orbit coupling for the t_{2g} orbitals.