TT 12: Correlated Electrons: Materials

Time: Tuesday 9:30–13:00 Location: H22

TT 12.1 Tue 9:30 H22

Low-dimensional magnetism in ordered perovskite and Ruddlesden-Popper variants — •Ryan Morrow, Anastasiia Smerechuk, Tamara Holub, Sabine Wurmehl, and Bernd Büchner — Leibniz Institute for Solid-State and Materials Research, IFW-Dresden, 01069 Dresden, Germany

Perovskites and their myriad of structural permutations have long been studied for their intriguing properties and interplay of degrees of freedom, both chemical and physical. While generally three dimensional in nature, perovskites can provide multiple means of access to low dimensional properties as well. In this talk, new results in three different directions pertaining to this concept will be presented. The first, most common approach, is the use of the Ruddlesden-Popper and similar phases, which separate perovskite-like layers with interlaced AO layers, rendering them primarily two dimensional. Several new cation-ordered iridate and rhodate Ruddlesden-Popper phases will be presented. The second approach is that of orbital order using Cu^{2+} in the double perovskite structure to yield in-plane only square lattice like magnetic interactions (e.g. Ba_2CuWO_6). New compounds produced by substitution series and high pressure methods will be shown. The third is that of vacancy ordering. By ordering of vacancies in combination with cation ordering, hexagonal perovskite phases can be reduced to well separated triangular two dimensional magnets with variable spin sizes and frustration. Again, new compounds will be shown. In all three directions, primarily crystallographic and magnetometry data on these new inorganic transition metal oxides will be presented.

TT 12.2 Tue 9:45 H22

Strain mediated phase transitions in $SrCrO_3$ — •Alberto Carta and Claude Ederer — Materials Theory, ETH Zurich, Switzerland

$SrCrO_3$ is a complex perovskite oxides that can exhibit a plethora of interesting and technologically promising characteristics. However, available experimental reports still disagree on whether the material is metallic or semiconducting, or whether it is paramagnetic or antiferromagnetic. In a recent pre-print, Bertino et al. also reported a transition from conducting to insulating behavior for thin films of $SrCrO_3$ grown at different levels of epitaxial strain [1]. In our work, we use density functional theory (DFT) and DFT+U to establish the basic properties of $SrCrO_3$. Our calculations clearly suggest a metallic C-type antiferromagnetic ground state, consistent with previous DFT studies[2]. Furthermore, we show that the electronic and magnetic properties of $SrCrO_3$ are strongly influenced by epitaxial strain, and that the system can develop orbital order coupled to a Jahn-Teller structural distortion under tensile strain. We explore the regime where this distortion is possible and propose a mechanism for the transition to the insulating state that is consistent with the observations of [1].

[1] G. Bertino, H.C. Hsing, A. Gura, X. Chen, T. Sauyet, M. Liu, C.Y. Nam, M. Dawber, arXiv: 2104.02738 (2021)
[2] K.W. Lee, W. E. Pickett, Phys. Rev. B 80, 1 (2009)

TT 12.3 Tue 10:00 H22

Thermodynamic Signatures of the Soliton Lattice in Single-Crystal $TbFeO_3$ — •Alexander Engelhardt[1], Johanna Jochum[2], Andreas Bauer[1], Andreas Erb[3], Astrid Schneidewind[4], and Christian Pfleiderer[1] — [1]TU München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany — [3]Walther-Meißner-Institut, Garching, Germany — [4]Forschungszentrum Jülich GmbH, Jülich Center for Neutron Sciences at MLZ, Garching, Germany

The properties of the orthorhombic perovskite $TbFeO_3$ originate from the interplay of a Tb and Fe magnetic sublattices, resulting in a complex magnetic phase diagram. Perhaps most remarkable, at low temperatures, a complex and anharmonic magnetic structure, a so-called magnetic soliton lattice, was identified by means of neutron scattering under magnetic fields up to 4 T [1]. Here, we report the single-crystal growth of $TbFeO_3$ using a combination of a solid-state reactions and optical float-zoning. Measurements of the magnetic ac susceptibility and the specific heat are characteristic of strong easy-plane magnetic anisotropy with two prominent magnetic phase transitions in zero magnetic field at 8 K and 3 K, consistent with the literature. By combining transverse-field ac susceptibility measurements with neutron scattering, we have determined the magnetic phase diagram. When a magnetic field is applied along the hard magnetic c axis, the soliton lattice may be traced up to 12 T, the highest field studied.

[1] S. Artyukhin et al., Nat. Mater. 11, 694 (2012)

TT 12.4 Tue 10:15 H22

Lattice dynamic of $LiReO_3$ across the continuous ferroelectric-like structural transition — •Ksenia Denisova[1], Peter Lemmens[1], Kantaro Murayama[2], Xiangyu Gu[2], Hiroshi Takatsu[2], Cedric Tassel[2], and Hiroshi Kageyama[2] — [1]IPKM, TU BS, Braunschweig, Germany — [2]Kyoto University, Kyoto, Japan

The observation of a ferroelectric instability in metallic $LiOsO_3$ [1] with strongly correlated electrons [2] has fueled an intense discussion on the origin of polar metallicity. A comparative Raman study [3] of the isostructural compound $LiReO_3$ reveals that the enlarged lattice parameters leads to softer Li vibrations and enhances fluctuations in the system. The phonon anomalies point to the phase transition at T=175 K with a crossover regime to temperatures as low as 140 K. The hysteresis in the temperature evolution of ReO_6 related modes as opposed to an abrupt softening of Li vibrations in the ferroelectric phase speaks in favour of a decoupling of polar degrees of freedom and itinerant electrons.

Work supported by the DFG EXC-2123-390837967 Quantum-Frontiers, DFG Le967/16-1, and DFG-RTG 1952/1.

[1] Y. Shi et al., Nat. Mater. 12, 1024 (2013)
[2] J.S. Zhou et al., PRB 104, 115130 (2021)
[3] F. Jin et al., PNAS 116, 20322 (2019)

TT 12.5 Tue 10:30 H22

Magnetic anisotropy, magnetoelastic coupling and the phase diagram of $Ni_{0.25}Mn_{0.75}TiO_3$ — •Ahmed Elghandour, Lukas Gries, Lennart Singer, Kaustav Dey, and Rüdiger Klingeler — Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany

Thermodynamic studies on high-quality single crystals of $Ni_{0.25}Mn_{0.75}TiO_3$ have been used to investigate magneto-structural coupling and to construct the magnetic phase diagram. Clear anomalies in the thermal expansion at the spin ordering and spin reorientation temperatures, T_N and T_R, evidence pronounced magneto-elastic effects. Notably, magnetic entropy is released mainly above T_N implying considerable short range magnetic order up to about $4T_N$. This is associated with a large regime of negative thermal expansion of the c axis. Both T_N and T_R exhibit the same sign of uniaxial pressure dependence which is positive (negative) for pressure applied along the b (c) axis. In addition, while our data indicate a glassy behaviour below $T^* \approx 3.7$ K, a significant amount of Ni^{2+} moments seems neither involved in long-range order not in the glassy state.

TT 12.6 Tue 10:45 H22

NMR investigations of a quasi-two-dimensional Heisenberg antiferromagnet under pressure — •F. Bärtl[1,2], D. Opherden[1,2], C. P. Landee[3], S. Molatta[1,2], J. Wosnitza[1,2], M. Baenitz[4], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Clark University, Worcester, Massachusetts, USA — [4]MPI for Chemical Physics of Solids, Dresden, Germany

The molecular-based material $[Cu(pz)_2(2\text{-}HOpy)_2](PF_6)_2$ (CuPOF) is an excellent realization of a two-dimensional square-lattice quantum $S = 1/2$ Heisenberg antiferromagnet, with an intralayer exchange coupling $J/k_B = 6.8$ K and an interlayer coupling $J' \approx 10^{-4}J$. Previously reported nuclear magnetic resonance (NMR) data revealed a low-temperature transition to a commensurate antiferromagnetic (AF) quasistatic long-range order (LRO), with a preceding crossover from isotropic Heisenberg to anisotropic XY behavior. We present further NMR studies of the low-temperature correlations in magnetic fields up to 7 T and temperatures down to 0.3 K. The application of hydrostatic pressure up to 10 kbar leads to a change of the interlayer coupling and, therefore, the magnetic correlations in the critical regime. The transition regime is probed by ^{1}H and ^{31}P spectroscopy and relaxometry, revealing a monotonic change of T_N with increasing pressure. The commensurate AF LRO below T_N persists at high pressures, as re-

vealed by a splitting of the ^{1}H NMR lines, stemming from the broken symmetry of the local spin polarizations in the LRO regime.

TT 12.7 Tue 11:00 H22

Electronic structure of $CeTAl_3$ (T=Ag, Au, Cu, Pd, Pt) studied with density functional theory — •André Deyerling[1], Andreas Bauer[1], Christian Franz[2], Marc A. Wilde[1], and Christian Pfleiderer[1] — [1]Physics Department, Technical University Munich, Garching, Germany — [2]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

The $CeTAl_3$ family (T=Ag, Au, Cu, Pd, Pt) is prototypical of strongly correlated electron systems with a large variety of different magnetic ordering phenomena [1,2,3,4], such as ferromagnetism in $CeAgAl_3$ and incommensurate antiferromagnetism in $CeAuAl_3$. Further, in $CeAuAl_3$ [5] and $CeCuAl_3$ [6] magnetoelastic hybrid excitations between crystal electric fields and phonons have been observed. The electronic structure, and in particular the role of the Ce–4f electron, is key for understanding the mechanism driving these phenomena. We report electronic structure calculations for selected members of the $CeTAl_3$ family, where the Ce–4f electrons are described either as being itinerant or localized using DFT or DFT+U, respectively. The results of our calculations treating the 4f electrons as localized are in good agreement with the experimental data available.

[1] C. Franz et al., J. Alloy. Comp. 668, 978 (2016)
[2] D.T. Adroja et al., Phys. Rev. B 91, 134425 (2015)
[3] M. Klipcera et al., Phys. Rev. B 91, 224419 (2015)
[4] M. Stekiel et al., arXiv:2106.08194 (2021)
[5] P. Čermák et al., Proc. Natl. Acad. Sci. 116, 6695 (2019)
[6] D.T Adroja et al., Phys. Rev. Lett. 108, 216402 (2012)

15 min. break

TT 12.8 Tue 11:30 H22

Charge-carrier properties near the bandwidth-controlled Mott transition in layered organic conductors probed by magnetic quantum oscillations — •Mark V. Kartsovnik[1], Sebastian Oberbauer[1,2], Shamil Erkenov[1,2], Werner Biberacher[1], and Natalia D. Kushch[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany

Despite the great amount of work devoted to the Mott metal-insulator transition (MIT), some key theoretical predictions in this field are still awaiting experimental verification. In particular, there is no clarity about the exact behavior of the quasiparticle mass renormalized by many-body interactions, or about the pseudogap formation in the metallic ground state close to the bandwidth-controlled first-order MIT. Here we address these issues by employing organic κ-type salts as exemplary quasi-2D Mott systems and gaining direct access to their charge carrier properties via magnetic quantum oscillations. We trace the evolution of the effective cyclotron mass as the conduction bandwidth is tuned very close to the MIT by means of precisely controlled external pressure. We find that the sensitivity of the mass renormalization to subtle changes of the bandwidth strongly exceeds the theoretical predictions and is even further enhanced upon entering the transition region where the metallic and insulating phases coexist. On the other hand, even at this very edge of stability of the metallic ground state its Fermi surface remains fully coherent.

TT 12.9 Tue 11:45 H22

Anisotropic quasiparticle life times and magnetotransport in the doped Hubbard model — •Niklas Witt[1], Erik van Loon[2], Sergey Brener[1], Mikhail Katsnelson[3], Alexander Lichtenstein[1], and Tim Wehling[1] — [1]University of Hamburg, Hamburg, Germany — [2]Lund University, Lund, Sweden — [3]Radboud University, Nijmegen, The Netherlands

The strange metal phase of high-temperature superconducting copper oxide (cuprate) materials exhibits several unconventional transport properties like T-linear resistivity that do not conform to a conventional Fermi liquid description. The crossover to a normal metal for large dopings and the origin of the anomalous electronic properties remain unsolved problems.

Recent transport measurements [1,2] suggest that two different charge sectors exist, one with coherent quasiparticle charge carriers and the other with incoherent non-quasiparticle excitations. Only the former contributes to transport, leading to a drop of the Hall carrier density for small doping. To examine this hypothesis, we study the hole-doped Hubbard model using complementary many-body methods from the weak- and strong-coupling limit. We demonstrate that a dichotomy of the scattering rates between charge carriers from different momentum regions emerges which can lead to the reduction of the Hall carrier density already in the framework of semiclassical Boltzmann theory.

[1] M. Culo et al., SciPost Physics 11 (2021)
[2] J. Ayres et al., Nature 595, 661 (2021)

TT 12.10 Tue 12:00 H22

Electron spin resonance studies on layered van-der-Waals magnets — •Joyal John Abraham[1,2], Yurii Senyk[1], Alexey Alfonsov[1], Yuliia Shemerliuk[1], Sebastian Selter[1], Saicharan Aswartham[1], Bernd Büchner[1,3], and Vladislav Kataev[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 Wurzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, D-01062

Magnetic van-der-Waals (vdW) materials are compounds in which the planes consisting of magnetic atoms are held by weak vdW bonds. With a striking advantage of mechanical exfoliation to produce atomically thin layers, they are considered as promising candidates for studying exotic quantum phenomena and device application. Here, we present the investigation of magnetic vdW single crystals $Mn_2P_2S_6$ and $MnNiP_2S_6$, using high field/frequency electron spin resonance. Frequency dependence of resonance field reveals a change of the anisotropy from easy-axis-like in the pure Mn compound to an easy-plane-like in the mixed compound. Temperature dependence of resonance field and linewidth for in-plane and out-of-plane orientations of magnetic field reveals a shift in resonance from the paramagnetic position even above the transition temperature (T_N). This could be indicative of the presence of quasi-static spin-spin short-range correlations and hence provides insight about magnetic dimensionality of the studied material.

TT 12.11 Tue 12:15 H22

Magnon excitations, spin-lattice coupling and the emerging anisotropic nature of short-range order in van-der-Waals ferromagnets — M. Jonak[1], J. Arneth[1], A. Elghandour[1], E. Waldendy[1], S. Spachmann[1], C. Koo[1], M. Abdel-Hafiez[2], S. Selter[3], S. Aswartham[3], and •Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Dep. of Physics & Astronomy, Uppsala University, Sweden — [3]IFW Dresden, Germany

CrI_3 and $Cr_2Ge_2Te_6$ are quasi-2D semiconducting van der Waals ferromagnets which evolve long-range order down to the single- or double-layer limit. Quantitative determination of magnetic anisotropy and spin-lattice coupling are crucial to further exploit these materials. We report ferromagnetic resonance studies in a broad frequency regime of 30 - 330 GHz and in magnetic fields up to 18 T and high-resolution capacitance dilatometry. Our data prove significant magnetoelastic coupling and provide quantitative values of the uniaxial pressure effects. Modelling the magnon branches in CrI_3 by means of a domain-based ferromagnetic resonance model provides the microscopic parameters such the anisotropy gap of 80 GHz at 2 K which remarkably remains finite at T_C and vanishes only above 80 K. In addition, we detect short-range magnetic correlations up to at least 160 K. Notably, the nature of the short-range correlations in CrI_3 changes, confirming the importance of spin-orbit coupling for the evolution of long-range ferromagnetism which develops from magnetically anisotropic short-range order.

TT 12.12 Tue 12:30 H22

Orbital order and nematic instability in the antiferromagnetic phase of $BaCoS_2$ — •Benjamin Lenz[1], Michele Fabrizio[2], and Michele Casula[1] — [1]Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC), Sorbonne University - CNRS - MNHN, Paris, France — [2]Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

We present evidence for a nematic instability in the antiferromagnetic insulating phase of $BaCoS_2$, which shows a Néel transition at a surprisingly high temperature of $T_N \sim 300$K. Based on *ab initio* simulations, we discuss several competing orders in terms of magnetic order, orbital composition and structural distortions to identify a set of nematic and orbital ordered states as possible candidates for the ground state. From these considerations we derive an effective spin-model of $J_1 - J_2$ type and discuss the consequences of the most probable, orbital ordered ground state for its parametrization. We finally identify a

driving mechanism which allows to explain the high Néel temperature by $\mathcal{C}_4$-symmetry breaking through orbital order and draw parallels to other quasi-2D materials such as pnictides.

TT 12.13 Tue 12:45 H22

Tuning the multiorbital Mott transition of $BaCoS_2$ — •Haneen Abushammala[1,2], Yannick Klein[1], and Andrea Gauzzi[1] — [1]IMPMC, Sorbonne University, 4, place Jussieu, 75005 Paris, France — [2]Institute for Experimental Physics IV, Ruhr-Universität Bochum, Germany

The quasi-2D $BaCoS_2$ system displays an unusual Mott state concomitant with a stipe-type antiferromagnetic (AFM) ordering at T_N=305 K in a square-lattice of Co^{2+}. Electron doping by partial Co/Ni substitution, or hydrostatic pressure drives the system into a paramagnetic and Fermi Liquid (FL) metallic phase. Interestingly, this metal-insulator transition (MIT) is not accompanied by any significant structural distortion, which offers ideal conditions to investigate the FL to non-FL crossover in a model square-lattice system in the regime of moderate electronic correlations typical of sulphides. In order to investigate the interplay between AFM order and Mott state, we have studied the effect of chemical pressure and hole doping on the AFM order by partially substituting Sr and K for Ba respectively. Contrary to the case of hydrostatic pressure, we find that chemical pressure significantly reduces T_N down to 240 K for a substitution level of 8 at%, corresponding to an effective pressure of 0.3 GPa. The K-substitution is found to induce similar suppression of the AFM order as compared to the Sr-substitution. However, its sizable value of Sommerfeld coefficient (5.7 mJ/mol.K^2) suggests a metallic state induced by hole doping. Studies on single crystals may unveil whether the metallic state induced by K-doping displays FL-properties.