TT 9: Correlated Magnetism – Low-Dimensional Systems

Time: Monday 15:00–18:15 Location: H33

TT 9.1 Mon 15:00 H33

Pressure and quantum magnetism: Insights from brochantite $Cu_4SO_4(OH)_6$ — •Victoria Ginga[1], Bin Shen[2], Ece Uykur[3], Nico Giordano[4], and Alexander Tsirlin[1] — [1]Felix Bloch Institute, University of Leipzig, Germany — [2]EP VI, EKM, University of Augsburg, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Germany

Brochantite $Cu_4SO_4(OH)_6$, a widespread natural copper sulfate mineral, exemplifies a low-dimensional quantum magnet due to its geometrically frustrated $S = 1/2$ Cu^{2+} chains. The crystal structure of brochantite ($P2_1/n$) consists of edge-sharing zigzag double chains forming corrugated sheets in the *ab*-plane, with dissimilar Cu-O-Cu bridges fostering complex magnetic interactions. Ferromagnetic ordering within the Cu1-Cu2 and Cu3-Cu4 chains coexists with antiferromagnetic coupling between the chains, thus creating a delicate balance that can be affected by external pressure. We show that brochantite develops antiferromagnetic ordering below $T_N \approx 6$ K at ambient pressure. High-pressure X-ray diffraction data show that the monoclinic structure of brochantite remains stable up to at least 33 GPa, but individual structural parameters and especially bond angles are modified by pressure, thus affecting magnetic frustration in the compound. Magnetization measurements under pressure reveal changes in the Neel temperature and in the position of the susceptibility maximum. Our findings highlight brochantite as a platform for studying the interplay of structural and magnetic properties under extreme conditions.

TT 9.2 Mon 15:15 H33

μSR-investigation of clinoatacamite $Cu_2Cl(OH)_3$ — •Carolin Kastner[1], Fabrice Bert[2], Thomas J. Hicken[3], Jonas A. Krieger[3], Hubertus Luetkens[3], Aaron Schulze[1], Dirk Menzel[1], F. Jochen Litterst[1], Leonie Heinze[4], Kirrily C. Rule[5], Anja U. B. Wolter[6], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Braunschweig, Germany — [2]SQM, Université Paris-Saclay, Orsay, France — [3]PSI, Villigen, Switzerland — [4]FZ Jülich GmbH, JCNS at MLZ, Garching, Germany — [5]ANSTO, Kirrawee, Australia — [6]IFW Dresden, Dresden, Germany

Interest in the natural mineral clinoatacamite $Cu_2Cl(OH)_3$ arose due to its chemical and structural relationship to herbertsmithite, a candidate material featuring a quantum spin liquid state on the kagome lattice. In clinoatacamite, the Cu^{2+} spins form a system of distorted kagome layers with three inequivalent antiferromagnetic in-plane couplings and weaker ferromagnetic interlayer exchange. This gives rise to a complex magnetic phase diagram which contains a sequence of magnetic transitions of unknown symmetry.

Here, we present a study of the magnetic phase diagram of single-crystalline clinoatacamite using muon spin spectroscopy (μSR) to gain insight into the microscopic details of the different magnetic phases. For our investigation, the natural, single-crystalline samples were extensively pre-characterized by magnetization and specific heat. We will discuss our findings in the context of the local site symmetry of the different Cu ions.

TT 9.3 Mon 15:30 H33

Complex magnetic excitations in the alternating ferro-antiferromagnetic chain vompound $Cu_2(OH)_3Br$ — •Kirill Povarov[1], Yurii Skourskii[1], J. Wosnitza[1,2], David Graf[3], Zhiying Zhao[4], and Sergei Zvyagin[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence ct.qmat, HZDR, Dresden — [2]Institut für Festkörper- und Materialphysik, TU Dresden — [3]National High Magnetic Field Laboratory, Tallahassee — [4]Fujian Institute of Research of Structure of Matter, Fujian

We report the intricate spectrum of magnetic excitations in the mixed-chain quantum magnet $Cu_2(OH)_3Br$. Electron spin resonance (ESR) measurements in the frequency range between 0.1 and 1 THz reveal two distinct types of excitations: Low-energy modes of antiferromagnetic resonance (AFMR), and a high-energy excitation multiplet. The latter was argued to stem from mixing between the spinons and magnons, based on the results of zero-field neutron spectroscopy [1]. Peculiarities of their behavior in magnetic fields up to 16 T are discussed.

This work was supported by the Deutsche Forschungsgemeinschaft through the Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter - *ct.qmat* (EXC 2147, project No. 390858490) and the SFB 1143, as well as by HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

[1] Zhang *et al.*, PRL **125**, 037204 (2020).

TT 9.4 Mon 15:45 H33

Synthesis and physical properties of the quasi-spin chain compound Li_2CuO_2 — •Ashiwini Balodhi[1,2] and Min Gyu Kim[2] — [1]Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, WI 53201, USA

Li_2CuO_2 serves as an excellent model system for investigating low-dimensional magnetism, owing to its simple $CuOi_4$ square planar coordination along the b-axis (orthorhombic structure). Previous studies on both polycrystalline and single-crystal samples have revealed an antiferromagnetic (AFM) transition at $T_N \sim 9$ K, accompanied by a canted AFM spin structure at T = 2.6 K. To probe the intrinsic magnetic properties of Li_2CuO_2, we synthesized this material using the flux method. We will present detailed magnetic, and heat capacity measurements on flux-grown samples. Magnetization and heat capacity data confirm a long-range antiferromagnetic transition at T_N = 9.3 K. In contrast to earlier studies reporting ferromagnetic components at low temperatures, our results do not indicate any evidence of ferromagnetic ordering in low temperature regime.

This work is supported by the University of Wisconsin-Milwaukee.

[1] A. Balodhi, M. G. Kim, Crystals 14, 288 (2024).
[2] A. Balodhi, M. G. Kim. J.Magn.Magn.Mater. 611, 172617 (2024).

TT 9.5 Mon 16:00 H33

Sub-Kelvin magnetic susceptibility insights into the spin chain system $YbAlO_3$ — •Lipsa Behera[1,2], Javier Landaeta[2], Konstantin Semeniuk[2], and Elena Hassinger[1,2] — [1]TUD Dresden University of Technology, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Low dimensional quantum magnets offer a rich platform to explore intriguing physics such as Tomonaga-Luttinger liquid, incommensurate phases and quantum phase transitions. What makes them special is the constraint in dimensionality leading to strong correlations. $YbAlO_3$ is an example of a quasi-one-dimensional spin chain system that can be described as a S = 1/2 Heisenberg chain with smaller Ising-like interchain interactions. At 1K it shows a typical spinon spectrum. At low temperature, the phase diagram presents an antiferromagnetic phase below 0.9 K, that changes into a longitudinal spin density wave including a MS/3 plateau, transverse antiferromagnetic phase and the field polarised state with H ||a. Recent thermal conductivity and magnetostriction measurements uncovered a previously unobserved MS/5 plateau phase at B = 0.7 T, motivating detailed sub-kelvin magnetic susceptibility studies. Here, we report ac susceptibility measurements down to 25 mK, which not only reproduces the known phase diagram to a good extent, but also confirm the presence of the magnetization plateau Ms/5. Furthermore, it reveals additional anomalies, embedded in the incommensurate phase, adding up to the complex magnetic behavior of this material.

TT 9.6 Mon 16:15 H33

Evidence of spin-phonon charge coupling in the quasi-1D Ising spin chain system α-CoV_2O_6 — •Debismita Naik and Pradip Khatua — Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, West Bengal 741246, India

The quasi-one-dimensional Ising spin chain system α-CoV_2O_6 exhibits fascinating magnetic properties at lower temperatures. The DC magnetization and specific heat confirm the antiferromagnetic long-range ordering temperature T_N = 15 K. From the specific heat, the calculated magnetic entropy above T_N suggests short-range ordering in this low-dimensional compound. The temperature-dependent XRD supports the key finding of magnetoelastic coupling, which is crucial for linking the electrical and magnetic dipoles. Temperature-dependent Raman spectroscopy reveals the presence of spin-phonon coupling below T_N. Additionally, the study highlights an unusual evolution of the Raman modes above T_N which appears to be linked to short-range magnetic ordering. The renormalization of Raman modes and lattice anomalies near T_N illustrate spin-lattice coupling via magnetoelastic and spin-phonon interactions leads to interplay between spin, charge, and phonon degrees of freedom in α-CoV_2O_6. To support the intriguing phenomena, the theoretical charge density difference maps suggest the formation of electrical dipoles between Co and O atoms below T_N arises from p-d hybridization.

15 min. break

TT 9.7 Mon 16:45 H33

Crystal structure, electronic structure and magnetism in the binary compound Cr_3Se_4 — •Helge Rosner[1], Seojin Kim[1], Yurii Prots[1], Vincent Morano[2], Oksana Zaharko[2], Jörg Sichelschmidt[1], Marcus Schmidt[1], and Michael Baenitz[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Laboratory for Neutron Scattering and Imaging, 5232 Villigen PSI, Switzerland

Cr_3Se_4 crystallises in a monoclinic lattice, structurally closely related to the rhombohedral chalcogenite delafossite-like systems $ACrX_2$ with A = Na, Cu, Ag and X = S, Se. In contrast to these intrinsically semiconducting materials with a nonmagnetic monovalent A site, in Cr_3Se_4 the distorted triangular $CrSe_2$ layers are separated by a formally trivalent and magnetic ion. In consequence, the inter-layer distance is strongly reduced, making the system more three dimensional, and thus strongly increasing the magnetic ordering temperature.
Here, we present a joint experimental and theoretical study of the binary material Cr_3Se_4, including thermodynamic measurements, high resolution XRD, neutron scattering and density functional band structure calculations. Our data consistently demonstrate that the metallic system undergoes an antiferromagnetic ordering at about 160 K which is strongly coupled to the crystal lattice. The band structure calculations show that the conduction bands originate from strongly hybridised Cr-Se states with sizeable spin-orbit interaction. In a detailed comparison, we will highlight the similarities and differences between Cr_3Se_4 and the chalcogenite delafossites.

TT 9.8 Mon 17:00 H33

First-principles phonon study of $AgCrS_2$, $AgCrSe_2$, and $AgCrTe_2$ — •Seo-Jin Kim, Jörg Sichelschmidt, Michael Baenitz, Yurii Prots, Markus Schmidt, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We study the elastic and dynamic stability of layered triangular lattice systems $AgCrS_2$, $AgCrSe_2$, and $AgCrTe_2$ using density functional theory (DFT). These systems share the same structure but exhibit different properties. Multiferroic $AgCrS_2$ undergoes an additional structural transition to a monoclinic phase and exhibits a collinear double-stripe antiferromagnetic ground state below $T_N = 42$ K. $AgCrSe_2$ shows noncollinear cycloidal magnetic ordering below $T_N = 32$ K. To investigate the interplay between magnetism and structure, we analyze the elastic constants and phonon dispersions of these compounds. Our findings reveal that the on-site Coulomb repulsion and additional symmetry alterations in the Cr layer are crucial for achieving dynamical stability in $AgCrS_2$. Furthermore, we analyze $AgCrSe_2$ and $AgCrTe_2$ to understand the general trends in elastic and dynamic properties with chalcogen variation.

TT 9.9 Mon 17:15 H33

Magnetic-field tuning of the spin dynamics in the van der Waals antiferromagnet $CuCrP_2S_6$ (CCPS) — •Joyal John Abraham[1,2], Sebastian Selter[1], Yuliia Shemerliuk[1,2], Saicharan Aswartham[1], Bernd Büchner[1,2,3], Vladislav Kataev[1], and Alexey Alfonsov[1] — [1]Leibniz IFW Dresden, D-01069 — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01062 Dresden — [3]Institute for Solid State and Materials Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, D-01062

Magnetic van der Waals (vdW) materials have recently attracted significant attention due to their tunable magnetic properties, easy exfoliation, and possible integration into spintronic devices. In this work, we explore with electron spin resonance (ESR) spectroscopy the spin dynamics of the vdW antiferromagnetic (AFM) compound CCPS featuring interpenetrating antipolar Cu^{1+} and (AFM) Cr^{3+} sublattices. Above the AFM ordering temperature $T_N \approx 30$ K ESR reveals prominent ferromagnetic (FM) spin correlations that persist far above T_N, suggesting an intrinsically two-dimensional character of the spin dynamics in CCPS. At $T < T_N$, a complex field dependence of collective excitations of the AFM-ordered spin-lattice was observed featuring two non-degenerate magnon gaps at $H = 0$. A remarkable tuning of the excitations from the AFM-type to the FM-type with increasing field strength was demonstrated. Application of the linear spin wave theory enabled us to quantify the exchange and anisotropic constants. Furthermore, this unusual crossover of AFM-FM excitations is explained using the obtained energy parameters.

TT 9.10 Mon 17:30 H33

Investigation of the insulator to metal transition in the 2d van der Waals magnet $FePSe_3$ — •Saicharan Aswartham, Masoumeh Rahimkhani, Andreas Kreyssig, and Anna Böhmer — Experimentalphysik IV, Ruhr- Universität Bochum, 44801 Bochum, Germany

Layered magnetic van der Waals (vdW) materials offers an interesting playground for the investigation of correlated electronic ground states in two dimensions. $FePSe_3$ belongs to the family of transition metal phosphorus trichalcogenides $TMPX_3$ with an antiferromagnetic ground state with T_N=108 K. Interestingly, under the application of external pressure FePSe3 undergoes insulator to metal transition. Here, we present detailed synthesis and physical properties of $Fe_{1-x}TM_xPSe_3$ with different transition metal substitution. We furtheraim to investigate spin cross over behaviour with the application of chemical pressure in $FePSe_3$.

[1] Wang et al., Nat. Commun. 9, 1914 (2018).
[2] Selter et al., Phys. Rev. Mater. 5, 073401 (2021).

TT 9.11 Mon 17:45 H33

Modelling low-energy spin excitation measurements in field-induced phases of the spin-ladder antiferromagnet $BiCu_2PO_6$ — Patrick Pilch[1], Kirill Amelin[2], •Gary Schmiedinghoff[3], Anneke Reinold[1], Changqing Zhu[1], Kirill Yu. Povarov[4], Sergei Zvyagin[4], Hans Engelkamp[5], Yin-Ping Lan[6], Guo-Jiun Shu[6], Fang-Cheng Chou[7], Urmas Nagel[2], Toomas Rõõm[2], Götz S. Uhrig[1], Benedikt Fauseweh[1,3], and Zhe Wang[1] — [1]TU Dortmund, 44227 Dortmund, Germany — [2]NICPB, 12618 Tallinn, Estonia — [3]DLR, 51147 Cologne, Germany — [4]HZDR, 01328 Dresden, Germany — [5]Radboud University, 6525 ED Nijmegen, The Netherlands — [6]Taipei Tech, Taipei 10608, Taiwan — [7]NTU, Taipei 10617, Taiwan

We report on terahertz spectroscopic measurements and subsequent theoretical modelling of quantum spin dynamics on single crystals of a spin-1/2 frustrated spin-ladder antiferromagnet $BiCu_2PO_6$ as a function of applied external magnetic fields. Anisotropic spin triplon excitations are observed, which split in applied magnetic fields with a quantum phase transition at $B_{c1} = 21.4\,T$ for fields applied along the crystallographic a axis.

We theoretically model the magnetic field dependence of the triplon modes by using continuous unitary transformations to determine an effective low energy Hamiltonian. Through an exhaustive parameter search we find numerically optimized parameters to very well describe the experimentally observed modes, which corroborate the importance of significant magnetic anisotropy in the system.

The talk focuses on the theoretical analysis of the experimental data.

TT 9.12 Mon 18:00 H33

Evidence of multiple phase transition in $Sr_2BB'O_6$ — •Aprajita Joshi, Shalini Badola, Akriti Singh, and Surajit Saha — Indian Institute of Science Education and Research Bhopal, India

The manifestation of phase transition is well mimicked by the lattice, thus by phonons, which requires its correlation with other degrees of freedom (spins, phonons etc.). Often, one can study the behavior of associated phonons with external perturbation to get more insight into the ground state of the material. Thus, any changes in the phase can be tracked with the external stimuli. Keeping this in mind, we explored the structural and magnetic attributes of $Sr_2BB'O_6$ with the help of Raman spectroscopy, using temperature as an external perturbation. The obtained phonon parameter shows the signature of a series of structural phase transitions. Magnetic measurements reveal that it also stabilizes in an antiferromagnetic ground state. An apparent deviation in Raman modes was seen around both the magnetic transitions, acting as a signature of spin-phonon coupling in the system. Additionally, temperature-dependent Raman gave insight into the local distortion in the lattice arising in the magnetically ordered state. This was also corroborated by temperature-dependent XRD measurements.