MA 5: Cooperative Phenomena and Phase Transitions (joint session MA/TT)

Time: Monday 9:30–13:15 Location: HSZ 401

MA 5.1 Mon 9:30 HSZ 401

Driving the magnetic transition by chemical substitution in $Cs_{1-x}Rb_xFeCl_3$ — •Lena Stoppel[1], Shohei Hayashida[1], Zewu Yan[1], Severian Gvasaliya[1], Andrey Podlesnyak[2], and Andrey Zheludev[1] — [1]Laboratory for Solid State Physics, ETH Zurich, Switzerland — [2]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennesse

We report the observation of a chemical-substitution driven phase transition from a gapped quantum paramagnetic phase to one with long range order in $Cs_{1-x}Rb_xFeCl_3$. The $x = 0$ compound in this series of triangular-lattice antiferromagnets has a spin-singlet ground state due to strong easy-plane magnetic anisotropy. In contrast, the $x = 1$ material orders magnetically in a 120° structure [1]. Calorimetric and magnetic experiments performed on a series of samples with $0 \leq x \leq 1$ reveal that in the low-temperature limit magnetic order appears at $x \sim 0.35$. Inelastic neutron scattering experiments show that this coincides with the closure of the gap in the spin excitation spectrum. It appears that disorder effects in this material are more pronounced than those in the only other known phase transition of this type, namely in DTNX [2].

[1] S. Hayashida L. Stoppel et al., Phys. Rev. B 99, 224420 (2019). [2] K. Yu. Povarov et al., Phys. Rev. B 92, 024429 (2015).

MA 5.2 Mon 9:45 HSZ 401

Lattice effects in pyrochlore compounds $A_2B_2O_7$ — •M. Doerr[1], T. Stoeter[1,2], S. Granovsky[1], S. Zherlitsyn[2], and J. Wosnitza[1,2] — [1]Institut für Festkörper- und Materialphysik, TU Dresden — [2]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf

The magnetic character of pyrochlores $A_2B_2O_7$ (A = rare earths, B = transition metals or p-elements, *e.g.* Ti, Zr, Hf, Sn) strongly depends on the lattice. The ionic radii determine their existence and stability. The question of whether the ground state is degenerated or magnetically ordered is decisively determined by the ratio of dipole and exchange interaction. We present investigations of thermal expansion, magnetostriction and relaxation processes at temperatures down to 0.05 K. $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ show a number of anomalies that can be explained with both exchange and crystal-field effects. These anomalies reflect as well the magnetic properties via magnetoelastic coupling. Thus, statements on the monopole dynamics can be derived from relaxation processes. Relaxation times in the order of 10^3 s evidence the formation and annihilation of monopoles in the kagome-ice and saturated phase, in accordance with the known magnetic phase diagram. In contrast, the lattice effects in $Dy_2Sn_2O_7$ and $Ho_2Sn_2O_7$ are rather negligible. At last, measurements on $Pr_2Zr_2O_7$, $Gd_2Zr_2O_7$ and $Nd_2Hf_2O_7$ allow the direct comparison of classical spin-ice compounds to pyrochlores with light rare earths. A representation-theoretic investigation of the symmetry group of the pyrochlore lattice could lead to a better understanding of the magnetoelastic coupling mechanisms.

MA 5.3 Mon 10:00 HSZ 401

Control of structure and physical properties of La0.7Sr0.3MnO3 thin films via oxygen stoichometry — Lei Cao[1], •Oleg Petracic[1], Paul Zakalek[1], Alexander Weber[2], Ulrich Rücker[1], Jürgen Schubert[3], Alexandros Koutsioubas[2], Stefan Mattauch[2], and Thomas Brückel[1] — [1]Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT Forschungszentrum Jülich GmbH, Jülich — [2]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ) Forschungszentrum Jülich GmbH, Garching — [3]Peter Grünberg Institute (PGI9-IT) JARA-Fundamentals of Future Information Technology Forschungszentrum Jülich GmbH, Jülich

Epitaxial thin films of La0.7Sr0.3MnO3 were prepared by high oxygen pressure sputter deposition on SrTiO3 substrates at various oxygen partial pressures. In addition, we performed after preparation systematic oxygen desorption and absorption studies by thermal annealing or oxygen plasma processing, respectively. We derive a phase diagram with respect to the crystal structure (Perovskite vs. Brownmillerite), the magnetic behavior (ferromagnetic vs. antiferromagnetic) and the transport properties (metallic vs. insulating) for various annealing conditions.

MA 5.4 Mon 10:15 HSZ 401

Spin-lattice coupling in a Yafet-Kittel ferrimagnetic spinel — •Atsuhiko Miyata[1,2], Hidemaro Suwa[3], Toshihiro Nomura[2], Lilian Prodan[4], Viorel Felea[2,4,5], Yurii Skourski[2], Joachim Deisenhofer[6], Hans-Albrecht Krug von Nidda[6], Oliver Portugall[1], Sergei Zherlitsyn[2], Vladimir Tsurkan[4,6], Joachim Wosnitza[2,5], and Alois Loidl[6] — [1]LNCMI, Toulouse, France — [2]HLD-HZDR, Dresden Germany — [3]University of Tokyo, Tokyo, Japan — [4]Institute of Applied Physics, Chisinau, Moldova — [5]TU Dresden, Dresden, Germany — [6]University of Augsburg, Augsburg, Germany

Since the discovery of ferrimagnetism in 1948, noncollinear ferrimagnets have been well studied in spinels, AB_2X_4. The key essence is the competition of magnetic exchanges within or between the two A and B lattices. Yafet and Kittel (YK) proposed a model for triangular-structure ground states. To realize unconventional ferrimagnetic structures beyond the YK model, one can consider that spontaneous lattice deformation will modulate these main antiferromagnetic exchanges, i.e., through a spin-lattice coupling mechanism. This kind of spin-lattice coupling mechanism, however, has not been taken into account in previous theoretical works on ferrimagnetic spinels.

In this talk, using ultrasound and magnetostriction results up to 60 T, magnetization measurements up to 110 T, and Monte Carlo calculations, we demonstrate that the spin-lattice coupling induces unconventional magnetic structures under magnetic fields in the YK spinel $MnCr_2S_4$.

MA 5.5 Mon 10:30 HSZ 401

Pressure and field tuning in low-dimensional metal-organic magnets — •Matthew Coak[1], Samuel Curley[1], David Graf[2], Jamie Manson[3], and Paul Goddard[1] — [1]University of Warwick, Coventry, United Kingdom — [2]National High Magnetic Field Laboratory, Tallahassee, FL, USA — [3]Eastern Washington University, Cheney, WA, USA

The 1D molecular magnet $Cu(pyz)(gly)ClO_4$ (gly = glycine, pyz = pyrazine) is an $S = 1/2$ dimer material with small enough exchange constants to address with accessible fields. The dimers are coupled antiferromagnetically, possessing a singlet-triplet energy-gap that can be closed upon application of an external magnetic field. When the Zeeman splitting of the degenerate triplet state initially closes the gap, the system passes through a quantum phase transition from a quantum-disordered ground state to a long-range XY-ordered phase. This excited triplet state can be described as a system of bosonic quasi-particles called 'triplons'. Under certain conditions, this triplon excited state maps onto a Bose-Einstein condensate of magnons; $Cu(pyz)(gly)ClO_4$, at ambient pressures, appears to conform to this picture.

We present our latest results in using hydrostatic pressure as a tuning parameter to control the inter- and intra-dimer exchange interactions and observing the effects on the temperature-field phase diagram.

MA 5.6 Mon 10:45 HSZ 401

Spin crossover in mechanically responsive Ni(II)-MOF-74 — •Dijana Žilić[1], Krunoslav Užarević[1], Senada Muratović[1], Bahar Karadeniz[1], Tomislav Stolar[1], Stipe Lukin[1], Ivan Halasz[1], Mirta Herak[2], Gregor Mali[3], Yulia Krupskaya[4], and Vladislav Kataev[4] — [1]R. Bošković Institute, Zagreb, Croatia — [2]Institute of Physics, Zagreb, Croatia — [3]National Institute of Chemistry, Ljubljana, Slovenia — [4]Leibniz IFW, Dresden, Germany

The metal-organic frameworks (MOFs) are the subject of intensive research not only due to potential applications but also due to unresolved magnetic properties. We present here very detailed study of structural and magnetic properties of Ni(II)-MOF-74 compound, investigated by powder X-ray diffraction, infrared and Raman spectroscopy, magnetization measurements, X-band and multifrequency high-field electron spin resonance and solid state nuclear magnetic resonance spectroscopy. Our results show that Ni-MOF-74 can be described as a zig-zag spin chain system with ferromagnetic intrachain and weaker antiferromagnetic (AFM) interchain interaction, with long-range AFM phase transition around 17 K. We also studied how desolvation and amorphization process can influence the chemical and physical properties of Ni-MOF-74. The observed strong differences in magnetic properties of amorphous Ni-MOF-74 were explained by spin crossover from high-spin to low-spin state of Ni(II) ions.

Supported by HRZZ (UIP-2014-09-4744 and IP-2018-01-3168) and DAAD-MZO projects "Magneto-structural correlations in molecular magnetic complexes studied by electron spin resonance spectroscopy".

MA 5.7 Mon 11:00 HSZ 401

Atomistic simulations of spin-state switching in multinuclear spin-crossover molecules — •Robert Meyer, Christian Mücksch, Juliusz A. Wolny, Volker Schünemann, and Herbert M. Urbassek — Physics Department & Research Center OPTIMAS, University Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany

Spin-crossover materials exhibit the unique ability to switch between a low-spin and a high-spin state, indicating their potential as possible organic storage devices. A switch between the low and the high spin state is reflected by a frequency shift in the phonon density of states. This makes the phonon density of states an interesting tool to analyze spin-crossover materials.

We use a molecular dynamics approach to calculate the phonon density of states for both spin states. In particular, we are interested in the spin-switch behaviour of multinuclear SCO-compounds. We report on spin-switch dynamics depending on chain-length and number of switched atoms.

MA 5.8 Mon 11:15 HSZ 401

Noncoplanar magnetic order induced absence of large anomalous Hall effects in Mn_3Sn — •Xiao Wang[1], Fengfeng Zhu[1], Junda Song[1], Yixi Su[1], and Thomas Brückel[2] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Jülich, Germany

Recent experimental realizations of large anomalous Hall effect (AHE) at room temperature[1] in the non-collinear antiferromagnet (AFM) Mn_3Sn have attracted strong interests on this compound due to its potential applications in antiferromagnetic spintronics devices. We have prepared high quality Mn_3Sn single crystals [2] and studied its physical properties and magnetic structure by various methods. Surprisingly, below a magnetic phase transition at 280 K, the AHE vanished completely along with the emergence of two incommensurate phases. Our further polarized neutron scattering studies show the low temperature magnetic structures are noncoplanar order. Based on the polarized analysis results, we propose several possible magnetic structure models below 280 K. Moreover, we will discuss the reason for disappearance of AHE in the low temperature noncoplanar structures with magnetic symmetry analysis[3] and scalar spin chirality theory.

[1] S. Nakatsuji, et al., Nature 527, 212 (2015). [2] N.H. Sung, et al., Appl. Phys. Lett. 112, 132406 (2018). [3] M.-T. Suzuki, et al. Phys. Rev. B 95, 094406 (2017).

MA 5.9 Mon 11:30 HSZ 401

Magnetic structures and interplay between Eu and Mn in Dirac material EuMnBi2 — •Fengfeng Zhu[1], Xiao Wang[1], Junda Song[1], Thomas Müller[1], Yixi Su[1], and Thomas Brückel[2] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Jülich, Germany

We report here a comprehensive determination of the antiferromagnetic (AFM) structures of Eu and Mn magnetic sub-lattices by using both polarized and non-polarized single-crystal neutron diffraction methods. All the magnetic moments are orientated along c axis, the magnetic propagation vector is (0,0,1) for Eu sub-lattice and (0,0,0) for Mn sub-lattice. With proper neutron absorption correction, the ordered moments are refined as about 7.7 μ_B and 4.1 μ_B for the Eu and Mn ions, respectively, at 3K. In addition, a spin-flop phase transition of Eu moments was confirmed at field $B_c \sim$5.3T along c axis which is constant with previous reported work [1] and the evolution of magnetic moment orientations were also determined. In the spin-flop process, we found a clear kink in the field dependence of magnetic diffraction (1,0,1) of Mn, which unambiguously indicates the existence of strong coupling between Eu and Mn moments [2].

[1] H. Masuda et al., Sci. Adv. 2, e1501117 (2016) [2] A. F. May et al., Phys. Rev. B 90, 075109 (2014)

MA 5.10 Mon 11:45 HSZ 401

Ferrimagnetism in $CeSb_2$: Measuring bulk magnetic properties with an STM — •Christopher Trainer[1], Paul Canfield[2], and Peter Wahl[1] — [1]University of St Andrews, School of Physics and Astronomy, St Andrews, Fife, UK — [2]Iowa state University, Department of Physics and Astronomy, Ames, Iowa, US

$CeSb_2$ is one of a family of rare earth magnetic materials that exhibit metamagnetism where the magnetic state can be changed by an applied magnetic field. At low temperature it exhibits a complex phase diagram with multiple magnetically ordered phases for many of which the order parameter is only poorly understood. In this talk I will report Scanning Tunneling Microscopy and magnetization measurements of $CeSb_2$. I introduce a new mode of STM measurements which allows for the characterization of the sample magnetostriction and thus the construction of a bulk phase diagram using an STM. From the magnetostriction measurement, we determine the bulk phase diagram and validate it by comparison with magnetization measurements. Our magnetostriction and magnetisation measurements indicate the low temperature ground state at zero field is ferrimagnetic. Quasiparticle interference mapping showing how the electronic behaviour develops through the phase diagram will also be discussed.

MA 5.11 Mon 12:00 HSZ 401

Spin-reorientation in CuCr2S4 from μSR — •Elaheh Sadrollahi[1,2], Jochen Litterst[2,3], Vladimir Tsurkan[4], and Alois Loidl[4] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institut für Physik der kondensierten Materie, Technische Universität Braunschweig, 38110 Braunschweig, Germany — [3]Centro Brasileiro de Pesquisas Físicas, 22290-180, Rio de Janeiro, RJ, Brazil — [4]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Muon Spin Relaxation and Rotation (μSR) experiments have been performed on the thio-spinel CuCr2S4 for further clarifying the long-standing controversy regarding its electronic and magnetic states [1,2]. Long regarded as ferromagnet (Tc=378 K) with magnetic moments residing only on Cr, CuCr2S4 is nowadays considered a ferrimagnetic with small magnetic moments on the Cu sites [3]. In addition to the transition at Tc, our μSR data reveal transitions around 50 K and 100 K with changes in spontaneous rotation signals and in relaxation behaviour. There is a close resemblance between these μSR results with those found for Fe1-xCuxCr2S4 with high Cu concentrations [4]. We interpret the transitions with spin re-orientations and will discuss Jahn-Teller effect as a possible reason. [1] F. K. Lotgering et al., J. Phys. Chem. Solids 30, 799 (1969) and Solid State Commun. 2, 55 (1964). [2] J. B. Goodenough, Solid State Commun. 5, 577 (1967) and J. Phys. Chem. Solids 30, 261 (1969). [3] A. Kimura et al., Phys. Rev. B 63,224420 (2001). [4] E. Sadrollahi, Doctoral Thesis (2018): https://publikationsserver.tubraunschweig.de/receive/dbbs_mods_00066058.

MA 5.12 Mon 12:15 HSZ 401

Epsilon iron as a spin-smectic state — Tommaso Gorni[1] and •Michele Casula[2] — [1]Laboratoire de Physique et d'Étude des Matériaux, École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Université Paris Sciences et Lettres, 75005 Paris, France — [2]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France

By first-principles and spin-model calculations, we study the high-pressure epsilon phase of iron. We reveal the existence of a modulated spin pattern, lower in energy than the previous results, where spin fluctuations lead to the formation of antiferromagnetic bilayers separated by null spin bilayers. This pattern is analogous to the smectic phase found in liquid crystals. The magnetic bilayers are likely orientationally disordered, owing to the soft interlayer excitations and the near-degeneracy with other smectic phases. This possible lack of long-range correlation agrees with neutron powder diffraction and could be integral to explaining its puzzling superconductivity.

MA 5.13 Mon 12:30 HSZ 401

Frustration induced highly anisotropic magnetic patterns in classical XY model on kagome lattice — •Alexei Andreanov[1] and Mikhail Fistul[1,2] — [1]IBS PCS, Daejeon, Korea — [2]Russian Quantum Center, Moscow, Russia

We predict and observed novel highly anisotropic magnetic patterns obtained in the classical *XY* model on kagome lattice. The frustration is provided by the presence of both ferromagnetic (FM) and antiferromagnetic interactions between adjacent magnetic moments. At a critical value of frustration $f_{cr} = 3/4$ the system exhibits a transition from the ferromagnetic state to highly-degenerated ground state. In this regime, $f_{cr} < f \leq 1$, the average magnetization $\langle \vec{M} \rangle \simeq N^{-1/4}$ (N is the number of spins). This scaling originates from highly anisotropic character of the groundstates with the FM ordering along the y-direction, and short-range correlations along the x-direction. These features are explained by the presence of the double-degenerate ground state in a single triangle of the kagome lattice supplied witg a large number of constraints. We anticipate the implementation of this model in various systems, e.g. natural magnetic molecular clusters, artificially prepared Josephson junctions networks, trapped-ions and/or photonic crystals.

MA 5.14 Mon 12:45 HSZ 401

Concept of geometrically controlling artificial magnetoelectric materials — •Oleksii M. Volkov[1], Ulrich K. Rössler[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum-Dresden-Rossendorf, Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V. (IFW Dresden), Dresden, Germany

Magnetoelectric materials combine coupled magnetic and electrical order parameters, that allowed to control magnetic states via electrical influence and vice versa [1]. This offers exciting prospectives for energy efficient memory, logic and sensor devices. Here, we propose a new approach to electric field controlled nanomagnets [2], where the manipulation of magnetic states is done geometrically via modification of mesoscale Dzyaloshinskii-Moriya interaction and curvature-induced anisotropy [3]. The concept refers to geometrically curved helimagnetic springs embedded in a piezoelectric matrix or sandwitched between two piezoelectric layers. The electric field induces tiny changes of geometrical parameters, that leads to the transition between homogeneous and periodic helimagnetic states. This results in the appearance of strong converse magnetoelectric effect (CME) 15×10^{-3} (A m^{-1})/(V m^{-1}), which is five times higher than CME for best laminated magnetoelectric composites 2.9×10^{-3} (A m^{-1})/(V m^{-1}).

[1] W. Eerenstein et al., Nature **442**, 759 (2006).
[2] O. Volkov et al., J. Phys. D: Appl. Phys. **52**, 345001 (2019).
[3] O. Volkov et al., Scientific Reports **8**, 866 (2018).

MA 5.15 Mon 13:00 HSZ 401

Orthomagnons and Quantum Weak Ferromagnetism in Kagome Antiferromagnets — •Robin R. Neumann[1], Alexander Mook[2], Jürgen Henk[1], and Ingrid Mertig[1,3] — [1]Institut für Physik, Martin-Luther-Universität, D-06120 Halle — [2]Department of Physics, University of Basel, CH-4056 Basel — [3]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle

Magnons are charge-neutral spin carriers that appear as excitations in magnetically ordered systems. The magnetic moment they carry is often thought to be antiparallel to the localized magnetic moments in the ground state, causing magnons in collinear (or coplanar) magnets to carry only those magnetic moment components offered by the texture.

In this talk, we lift the aforementioned limitation by introducing “orthomagnons,” whose magnetic moment has a component orthogonal to the magnetic texture. We demonstrate that the notion of orthomagnons appears naturally in coplanar antiferromagnets on the kagome lattice. As a consequence, both quantum and thermal fluctuations introduce a weak out-of-plane magnetic moment. In the limit of zero temperature, this gives rise to quantum weak ferromagnetism.