MA 4: Spin structures and magnetic phase transitions

Time: Monday 9:30–12:45 Location: EB 202

MA 4.1 Mon 9:30 EB 202

Nature of spiral state, electric polarisation and magnetic transitions in Sr-doped $YBaCuFeO_5$ from first-principles study — Dibyendu Dey[1], Snehasis Nandy[1], •Tulika Maitra[2], Chandra Shekhar Yadav[3], and Arghya Taraphder[1] — [1]Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur 721302, India — [2]Department of Physics, Indian Institute of Technology Roorkee, Roorkee -247667, India — [3]School of Basic Sciences, Indian Institute of Technology Mandi, Mandi 175001, India

The nature of the spiral magnetic state in type II multiferroic $YBaCuFeO_5$ has recently been a matter of debate. Using first-principles density functional theory (DFT) calculations within LSDA+U+SO approximation, we reveal the nature of spiral state and corresponding ferroelectric response in the incommensurate magnetic phase of $YBaCuFeO_5$. A helical spiral state with spins living in the ab-plane is found to be more stable. Owing to negligibly small Dzyaloshinskii-Moriya interaction and the absence of any spin current mechanism in the helical spiral state, electric polarization is predicted to be zero. These results are in good agreement with the recent single-crystal data. We further investigated $YBa_{1-x}Sr_xCuFeO_5$) in the entire range of doping x. A quantum Monte Carlo (QMC) calculation on an effective spin Hamiltonian with exchange interactions estimated from DFT calculations shows that the paramagnetic to commensurate phase transition temperature increases with doping till x=0.5 and decreases beyond consistent with experimental findings.

MA 4.2 Mon 9:45 EB 202

Magnetism in High-Pressure Iron — •Tommaso Gorni and Michele Casula — IMPMC, Univeristé Pierre et Marie Curie, Paris

Due to the high pressures involved, the vast majority of iron contained in the Earth's interior, from the upper mantle to the lower core, is found in the so-called ε-Fe phase, displaying an hcp structure and a lack of macroscopic magnetization. However, in the pressure range of 15-30 GPa, ε-Fe presents several fingerprints of an underlying magnetic state, among which superconductivity, believed to be mediated by antiferromagnetic fluctuations. First-principles simulations of paramagnetic and antiferromagnetic states both reproduce the experimental equation of state with a similar level of accuracy, whereas experimental evidence could not detect any magnetic splitting via Mössbauer spectroscopy on the one side, but suggested antiferromagnetic order via an anomalous Raman splitting on the other. Here, we perform a thorough re-investigation of the ε-Fe antiferromagnetic states by Density Functional Theory calculations, and we map our results onto a spin model that we solve via a classical Monte Carlo approach. We finally propose a new scenario where the long-range magnetic ordering is hampered by spins fluctuating in both amplitude and direction, as suggested by our first-principles calculations. Our results are supported by some very recent X-ray Emission Spectroscopy and Neutron Scattering data.

MA 4.3 Mon 10:00 EB 202

Comparison of diluted antiferromagnetic Ising models on frustrated lattices in a magnetic field — •Konstantin Soldatov[1], Alexey Peretyatko[1], Konstantin Nefedev[1], and Yutaka Okabe[2] — [1]Far Eastern Federal University, Vladivostok, Russia — [2]Tokyo Metropolitan University, Tokyo, Japan

We study diluted antiferromagnetic Ising models on kagome and triangular lattices in a magnetic field, using the replica-exchange Monte Carlo method. We observe five and seven plateaus in the magnetization curve of the diluted antiferromagnetic Ising model on the kagome and triangular lattices, respectively, when a magnetic field is applied. These observations contrast with the two plateaus observed in the pure model. The origin of multiple plateaus is investigated by considering the spin configuration of triangles in the diluted models. We compare these results with those of a diluted antiferromagnetic Ising model on the three-dimensional pyrochlore lattice in a magnetic field pointing in the [111] direction, sometimes referred to as the "kagome-ice" problem. We discuss the similarity and dissimilarity of the magnetization curves of the "kagome-ice" state and the two-dimensional kagome lattice.

MA 4.4 Mon 10:15 EB 202

Entropy of the diluted antiferromagnetic Ising models on the frustrated lattices using the Wang-Landau method — •Yuriy Shevchenko[1,2], Konstantin Nefedev[1,2], and Yutaka Okabe[3] — [1]School of Natural Sciences, Far Eastern Federal University, Vladivostok, Russian Federation — [2]Institute of Applied Mathematics, Far Eastern Branch, Russian Academy of Science, Vladivostok, Russian Federation — [3]Department of Physics, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan

We show the results of computer calculations of non-linear behavior of residual entropy on frustrated pyrochlore, triangular and kagome lattices.

Nonmonotonic zero-point entropy as a function of dilution concentration was observed experimentally and discussed in frames of generalization of Pauling's theory [Ke X. et al., Phys. Rev. Lett. 99, 137203 (2007)]. Motivated by the current interest in the pyrochlore lattice, we study the entropy of the diluted AFM Ising model on the frustrated lattices using the Wang-Landau algorithm, which directly calculates the energy density of states.

We also investigate other frustrated systems, the antiferromagnetic Ising model on the triangular lattice and the kagome lattice, demonstrating the difference in the dilution effects between the system on the pyrochlore lattice and that on other frustrated lattices, and discuss it's nonmonotonic behavior.

MA 4.5 Mon 10:30 EB 202

Optical study of vibronic coupling in the quantum spin liquid candidate Tb2Ti2O7 — •Evan Constable[1,2], R. Ballou[1], J. Robert[1], L Bergen[2], C. Decorse[3], J.-B. Brubach[4], P. Roy[4], E. Lhotel[1], V. Simonet[1], S. Petit[5], and S. deBrion[2] — [1]Institut Néel, CNRS and Université Grenoble Alpes, Grenoble, France — [2]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [3]ICMMO, Université Paris-Sud, Orsay, France — [4]Synchrotron SOLEIL, Gif-sur-Yvette, France — [5]Laboratoire Léon Brillouin, CEA, CNRS, Université Paris-Saclay, Gif-sur-Yvette, France

Vibronic coupling describes the interaction between electronic energy levels and phonon modes, often leading to a ground state that is considerably perturbed. In magnetic rare-earth pyrochlores (RE2Ti2O7, RE = Dy, Ho), large crystal field splitting of the electronic energy levels leads to exotic magnetic behaviour in the form of a highly degenerate spin ice ground state. The possibility that quantum fluctuations due to vibronic coupling could melt the spin ice state forming a quantum spin liquid, is an interesting prospect. It is thought that this process could be present in Tb2Ti2O7 as it does not appear to feature long range order nor a spin ice phase. Indeed, our investigations reveal favourable symmetry and energy conditions for vibronic coupling. Using optical spectroscopic techniques we find evidence of a hybridisation of crystal-field-phonon modes present across a broad temperature range. This vibronic process supports a collective state between the ground and excited levels, which provides a crucial path for quantum spin-flip fluctuations that inhibit the stabilisation of conventional magnetism.

MA 4.6 Mon 10:45 EB 202

Metamagnetic anomalies near dynamic phase transitions — •Patricia Riego[1,2], Paolo Vavassori[1,3], and Andreas Berger[1] — [1]CIC nanoGUNE, San Sebastian, Spain — [2]University of the Basque Country, Bilbao, Spain — [3]Ikerbasque, Bilbao, Spain

Ferromagnets that are subjected to an oscillating magnetic field H(t) can undergo a second order dynamic phase transition (DPT) at a critical period Pc, when the period P of H(t) becomes comparable to the intrinsic relaxation time of the system, which then gives rise to a non-vanishing period-averaged magnetization for P<Pc [1]. Decades of research have shown that the DPT belongs to the same universality class as the corresponding thermodynamic phase transition (TPT) that spin systems undergo as a function of temperature, and that both phase transitions exhibit equivalent properties close to the critical point [2,3]. In our detailed experimental and theoretical study, however, we find that the equivalency between DPTs and TPTs breaks down in the regime of slow critical dynamics [4]. Instead, we observe a dynamically disordered phase that exhibits metamagnetic anomalies that are absent in TPTs for equivalent spin systems. Furthermore, we show that the scaling regime of the DPT is significantly reduced, which has severely impacted all existing experiments on the DPT to date.

[1] T. Tomé and M. J. de Oliveira, Phys. Rev. A 41, 4251 (1990).

[2] G. Korniss, C. J. White, P. A. Rikvold, and M. A. Novotny, Phys. Rev. E 63, 016120 (2000). [3] A. Berger, O. Idigoras, and P. Vavassori, Phys. Rev. Lett. 111, 190602 (2013). [4] P. Riego, P. Vavassori, and A. Berger, Phys. Rev. Lett. 118, 117202 (2017).

MA 4.7 Mon 11:00 EB 202

Magnetism and H-T phase diagram of the C14 Laves phase Nb0.075Fe2.025 compound — •Stanislaw Dubiel[1] and Maria Balanda[2] — [1]AGH University of Science and Technology, Krakow, Poland — [2]Institute of Nuclear Physics, PAN, Krakow, Poland

A C14 Nb0.975Fe2.025 Laves phase compound was investigated aimed at determining the H-T magnetic phase diagram. Magnetization, M, and AC magnetic susceptibility measurements were performed. Concerning the former field-cooled and zero-field-cooled M-curves were recorded in the temperature range of 2-200K and in applied magnetic field, H, up to 1000 Oe, isothermal M(H) curves at 2 K, 5 K, 50 K, 80 K and 110 K as well as hysteresis loops at several temperatures over the field range from -10 to +10kOe. Regarding the AC susceptibility, both real and imaginary components were registered as a function of increasing temperature in the interval of 2 K - 150 K at the frequencies of the oscillating field from 3 Hz up to 999 Hz. An influence of an external DC magnetic field, H, on the temperature dependence of the AC suscpetibility was investigated, too. The measurements clearly demonstrated that the magnetism of the studied sample is weak, itinerant and has a reentrant character which is a novel observation. Based on the obtained results a magnetic phase diagram has been constructed in the H-T coordinates. The results have been validated in terms of the known models for the reentrant spin glasses.

15 minutes break

MA 4.8 Mon 11:30 EB 202

Magnetic characterization of the nanolaminated magnetic Mn_2GaC MAX phase — •Iuliia Novoselova[1], Ruslan Salikhov[1], Arni Ingason[2], Marina Spasova[1], Johanna Rosen[2], Ulf Wiedwald[1,3], and Michael Farle[1,4] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [2]Department of Physics, Linköping University, Linköping, Sweden — [3]National University of Science and Technology MISIS, Moscow, Russia — [4]Center for Functionalized Magnetic Materials, Immanuel Kant Baltic Federal University, Kaliningrad, Russia

Inherently nanolaminated $M_{n+1}AX_n$ (n=1,2,3) compounds - MAX phases - attract interest, since these materials provide unique anisotropic structural and physical properties [1]. Additionally, materials share properties associated with ceramics and metals [1]. The ternary Mn_2GaC MAX phase has been synthesized as a heteroepitaxial film with Mn as the exclusive M element [2]. We performed a comprehensive study of the temperature-dependent magnetization, magnetoresistive (MR) and magnetostrictive (MS) properties. The system exhibits complex antiferromagnetic states with spin-reorientation transition at T_t = 214 K. Large uniaxial MS of 450 ppm with sign inversion at T_t was observed. MS is accompanied by highly asymmetric MR up to 3% at B = 9 T [4]. This work is supported by DAAD 57214224 and DFG Grant SA 3095/2-1. [1] M. W. Barsoum, Prog. Solid State Chem. 28, 201 (2000). [2] A. S. Ingason et al., Mater. Res. Lett. 2, 89-93 (2014). [3] R. Salikhov, et al. J. Appl. Phys. 121, 163904 (2017). [4] Iu. P. Novoselova, et al. (under review).

MA 4.9 Mon 11:45 EB 202

The complex electronic phase diagram of single-crystalline R_2PdSi_3 (R = Ho, Dy) studied by thermal expansion and magnetostriction — •Liran Wang[1], Binh Tran[1], Mingquan He[2], Christoph Meingast[2], Mahmoud Abdel-Hafiez[3], Chongde Cao[4], Jens Bitterlich[5], Wolfgang Löser[5], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany — [3]Physikalisches Institute Goethe-Universität,Germany — [4]Department of Applied Physics, Northwestern Polytechnical University, P.R. China — [5]Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany

Thermal expansion and magnetostriction of single-crystalline R_2PdSi_3 (R=Ho,Dy) have been investigated by means of high-precision capacitance dilatometry and by specific heat studies. Pronounced anomalies in the uniaxial thermal expansion coefficients α_a and α_c and in the specific heat c_p mark the onset of long-range AFM order. The different nature of the ground states in both materials is concluded from signs of the thermal expansion anomalies, i.e., opposite uniaxial pressure dependencies. In both materials, there are Schottky-like anomalous entropy and anisotropic length changes which are attributed to crystal field effects and reorientation of the easy magnetic axes. The low-T magnetic phase diagrams and the magnetostriction data imply an interplay of single-ion effects and magnetic exchange interaction. Even small magnetic fields yield ferrimagnetic phases via yet unknown intermediate AFM (Dy_2PdSi_3) and ferrimagnetic (Ho_2PdSi_3) phases.

MA 4.10 Mon 12:00 EB 202

Symmetry and Spin Reorientation in Low-Dimensional Antiferromagnet $SeCuO_3$ — •Mirta Herak[1], Nikolina Novosel[1], William Lafargue-dit-Hauret[2], Xavier Rocquefelte[2], Željko Rapljenović[1], Martina Dragičević[1], and Helmuth Berger[3] — [1]Institute of Physics, Bijenička c. 46, HR-10000 Zagreb, Croatia — [2]Institut des Sciences Chimiques de Rennes UMR 6226, Université de Rennes 1, 35042 Rennes Cedex, France — [3]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We study the antiferomagnetic ground state of low-dimensional $SeCuO_3$ by combining torque magnetometry with simple phenomenological approach to magnetic anisotropy and Density Functional Theory (DFT) calculations. Combining measured torque data with phenomenological approach allows us to choose between several symmetry allowed shapes of magnetic anisotropy energy (MAE) and to determine spin orientation in zero and finite magnetic field. Results obtained in magnetic fields larger than spin-flop field indicate that spin reorientation is more complicated than usual spin flop found in collinear antiferromagnet. The microscopic origin of MAE in $SeCuO_3$ was also investigated theoretically, based on DFT+U calculations including spin-orbit coupling on an antiferromagnetic model. It was evidenced inequivalent copper sites impact differently the magnetic anisotropy of this system, leading to a change of the easy magnetization axis. This work is fully supported by the HrZZ grant UIP-2014-09-9775 and by the COGITO project "Theoretical and experimental study of magnetic and multiferroic materials".

MA 4.11 Mon 12:15 EB 202

Higgs mode and its decay in a two-dimensional antiferromagnet — Anil Jain[1,2], •Maximilian Krautloher[1], Juan Porras[1], Gihun Ryu[1], D.P. Chen[1], Douglas Abernathy[3], Jitae Park[4], Alexandre Ivanov[5], Jiri Chaloupka[6], Giniyat Khaliullin[1], Bernhard Keimer[1], and B.J. Kim[1,7] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai — [3]Quantum Condensed Matter Division, ORNL — [4]Heinz Maier-Leibnitz Zentrum, TU München — [5]Institut Laue-Langevin, Grenoble — [6]Central European Institute of Technology, Masaryk University, Kotlářská — [7]Department of Physics, Pohang University of Science and Technology

In recent years significant research has focused upon emergent behavior arising from a convergence of spin-orbit coupling (SOC) and strongly correlated electron interaction energies in $4d$ and $5d$-electron transition metal oxides. We have concentrated our investigation on Ca_2RuO_4, a layered 2D antiferromagnet. Mixing of the cubic crystal field and SOC results in a nominally non-magnetic pseudospin $\tilde{J} = 0$ state, which contrasts with experimental findings. To resolve this issue G. Khaliullin (PRL **111**, 197201 (2013)) proposed a mechanism where magnetically active transitions between the $\tilde{J} = 0$ singlet and higher energy $\tilde{J} = 1$ triplet are enabled by virtue of superexchange interactions, resulting in *excitonic magnetic* order. Here we present inelastic neutron scattering results that illustrate a key signature of this ground state – the presence of a longitudinal mode (or Higgs mode) that corresponds to length fluctuations of $\tilde{J}$.

MA 4.12 Mon 12:30 EB 202

Time-resolved nuclear resonance scattering experiments on spin crossover complexes — •Sakshath Sadashivaiah[1], Kevin Jenni[1], Andreas Omlor[1], Christina-Sophie Müller[1], Lena Scherthan[1], Marcus Herlitschke[2], Ilya Sergeev[2], Hans-Christian Wille[2], Ralf Röhlsberger[2], Juliusz Wolny[1], and Volker Schünemann[1] — [1]Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Deutsches Elektronen synchrotron (DESY), 22607 Hamburg, Germany

The high spin (HS) - low spin (LS) phase transition in laser excited spin crossover complexes occurs though an intermediate state of cooperative lattice vibrations. The mechanism is debated because the phonon density of states (DOS) is only partially accessed in previous studies such as Raman scattering or reflectivity [1]. Through time-resolved Nuclear Inelastic Scattering (NIS) experiments, we study the full DOS of the ground and excited states at 100 K in the [Fe(PM-BIA)$_2$(NCS)$_2$] complex using 14.4 keV synchrotron radiation (SR) pulses. The sample was excited by time-delayed laser pulses derived from a 531 nm source, which was triggered at every alternate SR pulse. By performing NIS (and Nuclear forward scattering) using the SR pulses accompanying the laser pulses, we measured the excited state [2]. The alternate SR pulses probe the ground state. We follow the effect of the laser pulses by comparing the resulting spectra with the static HS and LS spectra.

[1] R. Bertoni et al, *Nat. Mater.* **15**, 606 (2016).
[2] S. Sakshath et al, *Hyperfine Interact.* **238**, 89 (2017)