MA 9: Cooperative phenomena: Spin structures and magnetic phase transitions

Time: Monday 15:00–17:00 Location: H53

MA 9.1 Mon 15:00 H53

Linearly coordinated Ni in the two-dimensional quantum magnet K_2NiO_2 — •Tanita J. Ballé, Laurin Brunner, Alexander A. Tsirlin, and Anton Jesche — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86135 Augsburg, Germany

A huge magnetic anisotropy and the highest known coercivity field of more than 11 T are observed in $Li_2[Li_{1-x}Fe_x]N$, one of the scarce rare-earth free hard magnets. In this compound an unquenched orbital moment is manifested, enabled by the perfect linear, twofold coordination of iron between nitrogen, that gives rise to these properties [1]. In order to investigate the limits in exploiting this geometrical motive to achieve stable magnetic moments, we investigated similar compounds [2]. We will discuss the magnetic properties of a new member of this series: K_2NiO_2 that contains nickel in linear, twofold coordination between oxygen.

Field- and temperature dependent measurements of the Magnetization were performed, complemented by heat capacity data. Density functional theory revealed moderately enhanced orbital contributions to the magnetic moment of nickel. The magnetic susceptibility was calculated in a Heisenberg model and is in reasonable agreement with experiment.

[1] A. Jesche *et al.* Nat. Commun. **5**:3333. doi: 10.1038/ncomms4333 (2014)

[2] P. Höhn, TJB *et al.* Inorganics 4, **42** (2016)

MA 9.2 Mon 15:15 H53

Structural and magnetic properties of the compounds of the series $Mn_{5-x}Fe_xSi_3$ (x=1,2,3) — •Mohammed Ait haddouch, Jörg Voigt, Nicolo Violini, Karen Friese, Jörg Persson, and Thomas Brückel — Jülich Centre for Neutron Science-2/Peter Grünberg Institut-4, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The magnetic and the structural properties of the members of the $Mn_{5-x}Fe_xSi_3$ series with x=1,2,3 are investigated macroscopically and with diffraction methods to reexamine their structural and magnetic phase diagram using single crystalline specimen. Similar to the parent compound Mn_5Si_3, the compounds with x=1, 2, exhibit two antiferromagnetic phase transitions AF1 and AF2. In Mn_5Si_3 an inverse magneto-caloric effect is related to the transition from AF1→ AF2. The inverse magnetocaloric effect has been assigned to a transition from a spin wave excitation spectrum to a fluctuation dominated excitation spectrum when the magnetic structure is changed by application of an external magnetic field [1]. We are now interested in the changes of the magnetic structure if Mn is replaced by Fe. We present the similarities and differences when compared to the undoped parent compound and try to explain the transition from the AF structure found for low Fe content to an FM structure found at large Fe(x > 3) content.

[1] N. Biniskos et al, PHYS REV LET 120,257205 (2018)

MA 9.3 Mon 15:30 H53

Weak ferromagnetism in Mn_3X (X=Sn, Ge, Ga) compounds — •Bendegúz Nyári[1], András Deák[1,2], Jerome Jackson[3], and László Szunyogh[1,2] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]MTA-BME Condensed Matter Research Group, Budapest, Hungary — [3]STFC Scientific Computing Department, Warrington, UK

The intermetallic compounds Mn_3X (X=Sn, Ge, Ga) in hexagonal crystal structure show complex magnetic behavior. Neutron diffraction [1] and theoretical [2,3] studies reveal that these compounds have a triangular spin configuration displaying weak ferromagnetic deformation. In this work, we investigate theoretically the noncollinear magnetic structures of these compounds. Spin model parameters are obtained by using a spin-cluster expansion (SCE) technique. A model based on three magnetic sublattices allows both a group theoretical analysis and also a quantitative description of weak ferromagnetism. We also perform unconstrained and constrained LSDA calculations, where we focused on exploring the effect of spin-orbit coupling and induced moments. In case of Mn_3Sn, neutron diffraction experiments also reveal a helical modulation of the weak-ferromagnetic state along the z-axis not yet explained theoretically. We present detailed investigations on how these helical states appear in the isotropic Heisenberg model.

[1] S. Tomiyoshi *et al.*, J. Magn. Mater. 54–57, 1001 (1986)

[2] L. M. Sandratskii and J. Kübler, Phys. Rev. Lett. 76, 4963 (1996)

[3] D. Zhang *et al.* J. Phys.: Condens. Matter **25** (2013)

MA 9.4 Mon 15:45 H53

Electronic properties and spin waves of Mn5Si3 from first principles — •Flaviano José dos Santos[1], Nikolaos Biniskos[2,3], Manuel dos Santos Dias[1], Karin Schmalzl[2], Stefan Blügel[1], Stéphane Raymond[3], and Samir Lounis[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Jülich, Germany — [2]Jülich Centre for Neutron Science, Forschungszentrum Jülich, Outstation at ILL, Grenoble, France — [3]Université Grenoble Alpes, CEA, INAC, MEM, Grenoble, France

Mn5Si3 is an antiferromagnet hosting rich physics, such as the inverse magnetocaloric effect [1] and a large anomalous Hall effect [2]. However, many questions remain unanswered [3-4], such as why some Mn magnetic moments vanish in its collinear phase, what is the role of spin fluctuations and what is the minimal magnetic model hamiltonian. We tackle some of these problems with DFT calculations using the full-potential Korringa-Kohn-Rostoker method including spin-orbit coupling. We investigated the electronic and magnetic properties of the system in different magnetic phases, also determining the magnetic exchange interactions and the magnetocrystalline anisotropy. We used a scheme for spin waves in noncollinear magnets [5] to compute the spin-wave energies as a function of the external magnetic field. Our theoretical results, with a single free parameter, are in good agreement with experimental data from neutron scattering. – [1] Biniskos et al., PRL 120, 257205(2018). [2] Sürgers et al., Sci. Rep. 7, 42982(2017). [3] Silva et al., JPCM 14, 8707(2002). [4] Gottschilch et al., J. Mater. Chem. 22, 15275(2012). [5] Dos Santos et al., PRB 97, 024431(2018).

MA 9.5 Mon 16:00 H53

Photo-induced excitation and its relaxation in the magnetic and polaronic microstructure of a manganite studied by Ehrenfest dynamics — •Sangeeta Rajpurohit[1], Michael ten Brink[1,2], and Peter Blöchl[1,2] — [1]Institute for Theoretical Physics, Technical University Clausthal, Germany — [2]Institute for Theoretical Physics, Universität Göttingen, Germany

With several recent experimental observations of the long-lived excited states, manganites are seen as promising candidates for the future energy devices. The theoretical understanding of relaxation process in the strongly correlated manganites by investigating the interplay of the charge, spin and lattice degrees is of great interest. A microscopic model, extracted from the first-principles calculations, is proposed to analyse the electronic, atomic and magnetic microstructure of the manganites. The model is used within the framework of the Ehrenfest-like dynamics to study the evolution of the photo-excited system. The time-dependent Schrodinger equation is adopted for the evolution of the electron wave functions and spin degree of freedom while the atoms are treated classically. The relaxation timescale and pathway in the photo-excited $Pr_{0.5}Ca_{0.5}MnO_3$, notably, depend on the light-pulse intensity. In the weak intensity case, the electronic sub-system relaxes through an ultrafast lattice-assisted conical intersection process. The spin dynamics on the sub-picosecond timescale plays a crucial role, besides lattice dynamics, if the system is subjected to a high-intensity light pulse. Interestingly, a new long-lived excited-state, exhibiting phase-separation, emerges at an intermediate light-pulse intensity.

MA 9.6 Mon 16:15 H53

Magnetic properties of novel Rare-Earth Molybdenum oxides — •Kseniia Denisova[1,2,3], Anna Shlyakhtina[4], Mahmoud Abdel-Hafiez[5], Maxim Avdeev[6], Peter Lemmens[2,3], Olga Volkova[1], and Alexander Vasiliev[1] — [1]Dept. of Phys., MSU, Moscow, Russia — [2]IPKM, TU-BS, Braunschweig, Germany — [3]LENA, TU-BS, Braunschweig, Germany — [4]SICP, Moscow, Russia — [5]CHPSTAR, Beijing, China — [6]ANSTO, Bragg Inst., NSW, Australia

Compounds with the general formula $Ln_6MoO_{12-\delta}$ attract attention as they contain both transition and rare-earth elements. Heavy rare-

earth molybdenum oxides may crystallize in two different defect fluorite structures, i.e., cubic and rhombohedral ones [1,2]. The systematic experimental study of these series reveals that $Ln_6MoO_{12-\delta}$ in both structural modifications exhibit magnetism largely influenced by deviation from stoichiometry [3]. Supported by DFG-LE967/16-1, NUST "MISiS" Grant No. K2-2017-084 and RFBR project 16-03-00463a. [1] Schildhammer, et al., Chem. Mater. 28, 7487 (2016). [2] Shlyakhtina, et al., J. Mater. Chem. A 5, 7618 (2017). [3] Denisova, et al., J. Alloys and Comp. 778, 756 (2019).

MA 9.7 Mon 16:30 H53

Competition between Kondo and Kitaev Physics in a frustrated impurity coupled to a fermionic bath — •Tathagata Chowdhury, Ralf Bulla, and Achim Rosch — University of Cologne, Germany

Geometrically frustrated quantum impurities coupled to metallic leads have been shown to exhibit rich behavior with a quantum phase transition separating Kondo screened and local moment phases. Frustration in the quantum impurity can alternatively be introduced via Kitaev-couplings between different spins of the impurity cluster. We use the Numerical Renormalization Group (NRG) to study a range of systems where the quantum impurity comprising of a Kitaev cluster is coupled to a bath of non-interacting fermions. We characterize the ground state and intermediate unstable fixed points of the system in terms of the plaquette fluxes and determine the temperature dependence of the various crossover scales of the model. We also show that the model can be mapped at low temperatures to an effective two-impurity Kondo model.

MA 9.8 Mon 16:45 H53

Magnetism and magneto-elastic coupling in $LiFePO_4$ — Johannes Werner[1], Sven Sauerland[1], Changhyun Koo[1], Mahmoud Abdel-Hafiez[1,2], Christoph Neef[1], Sergei Zvyagin[3], and •Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany — [2]Physikalisches Institut, Goethe Universität, Frankfurt a.M., Germany — [3]High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

We report thermal expansion, magnetostriction, specific heat, static and pulsed-field magnetisation, and antiferromagnetic resonance studies on single-crystalline $LiFePO_4$ [1]. The evolution of long-range antiferromagnetic order at $T_N = 50.1(5)$ K which is associated with a significant magnetoelectric effect [2] features pronounced anomalies in the thermal expansion coefficients. Uniaxial pressure effects are positive for pressure along the a- and b-axes and only very small for p_c. This behaviour as well as anomalies in α appearing upon further cooling are discussed considering coupling of spin, structure, and dielectric properties. The magnetic phase diagram is mapped out. It features a spin-flop transition at $B\|b = 32$ T. Pulsed-field ESR experiments show closing of the AFM gap at B_{SF}. The AFM resonance modes are well described by a mean-field model employing orthorhombic anisotropy, DM interaction, and the excitation gap inferred from recent neutron data [3].

[1] C. Neef et al., J. Cryst. Growth 462, 50 (2017)
[2] R. Toft-Petersen et al., Phys. Rev. B 92, 024404 (2015)
[3] Y. Yiu et al., Phys. Rev. B 95, 104409 (2017)