MA 4: Magnetic Heusler Compounds and Complex Magnetic Oxides

Time: Monday 9:30–12:30 Location: EB 107

MA 4.1 Mon 9:30 EB 107

Impact of *d-d* hybridization on the magnetic and vibrational properties of Ni(-Co)-Mn-Ti: Comparison with *p-d* Ni-Mn-(In,Sn) — •Olga Miroshkina[1], Benedikt Eggert[1], Johanna Lill[1], Benedikt Beckmann[2], David Koch[2], Katharina Ollefs[1], Franziska Scheibel[2], Wolfgang Donner[2], Oliver Gutfleisch[2], Heiko Wende[1], and Markus E. Gruner[1] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Technical University of Darmstadt, Darmstadt, Germany

All-*d*-metal Heusler alloys are a new class of promising magnetocaloric materials for magnetic cooling devices. We study the effect of *d-d* hybridization on the magnetic and vibrational properties of Ni(-Co)-Mn-Ti in the framework of density functional theory. To retrieve traces of *d-d* orbital hybridization in L_3-edge spectra, we compare calculated densities of states and x-ray absorption spectroscopy with the case of Ni-Mn-(In,Sn). In our recent studies for Ni-Mn-(In,Sn) [1, 2], we have shown that *p*-element concentration, together with positional disorder, indirectly affects the magnetic exchange between the 3*d*-metal atoms. This can be employed to control the magnetization of the transition metal sublattice. Comparison of Ni(-Co)-Mn-Ti with the Ni-Mn-(In,Sn) allows us to reveal the impact of *d*-element on magnetic characteristics. We show how the interatomic hybridization in all-*d*-metal Heusler compounds can be exploited as an intrinsic tuning parameter to design high-performance magnetocaloric materials.

[1] F. Cugini *et al.*, *Phys. Rev. B* **105**, 174434 (2022).
[2] O. Miroshkina *et al.*, *Phys. Rev. B* **106**, 214302 (2022).

MA 4.2 Mon 9:45 EB 107

Exploring non-collinear ground states in Mn_2RhSn and Mn_2IrSn Heusler Magnets — •Jorge Cardenas-Gamboa[1], Rebeca Ibarra[1], Paul McClarty[2], Markou Anastasios[3], Edouard Lesne[1], Maia Vergniory[1,4], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Physics Department, University of Ioannina, 45110 Ioannina, Greece — [4]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain

Non-collinear magnetism has emerged as a fundamental and experimentally intriguing aspect of magnetism as one of the most non trivial aspects because of novel topological spin textures (skyrmions) and its potential applications in spintronic devices. Experiments on Mn_2RhSn have reported an unusual ground state with magnetic canting and a temperature-induced transition into the collinear ferrimagnetic mode.

In this work, we employ first-principles calculations to implement a mean-field approximation of the ground state in Mn_2RhSn and Mn_2IrSn compounds. This computational approach aims to provide deeper insights into exchange interactions and the magnetic orientation behaviour observed in the experiments.

MA 4.3 Mon 10:00 EB 107

Investigation of the relationship between structural, magnetic and electrical transport properties of $Mn_2Rh_{1-x}Ir_xSn$ epitaxial Heusler thin films: experiments and theory — •Edouard Lesne[1], Rebeca Ibarra[1], Jorge Cardenas[1], Paul A. McClarty[2], Maia G. Vergniory[1], Anastasios Markou[1,3], and Claudia Felser[1] — [1]Max-Planck-Institute für Chemische Physik fester Stoffe, Dresden, Germany — [2]Max-Planck-Institute für Physik komplexer Systeme, Dresden, Germany — [3]Physics Department, University of Ioannina, Ioannina, Greece

The noncentrosymmetric $Mn_2Rh_{1-x}Ir_xSn$ Heusler system which exhibits a noncollinear ferrimagnetic groundstate and is characterized by a D_{2d} symmetry has been in the focus of attention since the independent observation of magnetic skyrmion (Sk) and antiskyrmion (aSk) quasiparticles by real-space imaging techniques, and further inferred from their topological electrical transport footprint to the Hall effect.

Here we investigate the intertwined structural, magnetic, and electrical transport properties of the compositional series $Mn_2Rh_{1-x}Ir_xSn$ epitaxial thin films (with: $0 \leq x \leq 0.4$) grown by magnetron sputtering. In particular we report on an unusual nonmomotonic and sign-changing temperature dependence of the anomalous conductivity (AHC) in all investigated samples. Our results are discussed in light of a combined tight-binding, density functional and mean-field theory approach, which predict the magnetic groundstate of the system and the magnitude of the intrinsic part of the AHC.

MA 4.4 Mon 10:15 EB 107

The role of correlated Jahn-Teller polarons in the dynamics of laser-induced insulator-metal transitions — Tim Titze[1], Maximilian Staabs[1], Pia Henning[1], Karen Stroh[1], Stefan Mathias[1,2], Vasily Moshnyaga[1], and •Daniel Steil[1] — [1]Universität Göttingen, I. Physikalisches Institut, 37077 Göttingen, Germany — [2]Universität Göttingen, International Center for Advanced Studies of Energy Conversion (ICASEC), 37077 Göttingen, Germany

We explore the roles of the transition order and phase separation on quasiparticle and spin dynamics in colossal magnetoresistive $(La_{0.6}Pr_{0.4})_{0.7}Ca_{0.3}MnO_3$ (LPCMO) and $La_{0.7}Ca_{0.3}MnO_3$ (LCMO) thin films. LPCMO with a 1^{st} order phase transition is characterized by a strongly nonthermal, metastable response after nanosecond pulsed optical excitation close to the metal-insulator transition, leading to short-term transient metallization and a long-term conductivity decrease. The dynamics in LCMO (2^{nd} order phase transition) are dominantly thermally driven and show a fast recovery of the ground state. Our results highlight that the order of phase transition and the related nanoscale phase separation (JT polarons) play a crucial role for the persistence of laser-excited states in otherwise similar compounds.

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MA 4.5 Mon 10:30 EB 107

Quasi two dimensional antiferromagnetism in square planar iridate $Cs_2Na_2IrO_4$ — •Roumita Roy[1] and Sudipta Kanungo[2] — [1]Indian Institute of Technology Goa, India — [2]Indian Institute of Technology Goa, India

The study of iridates has gained major attention in recent times, as it is a promising candidate to study the the delicate interplay amongst competing energy scales. However the constant focus has been on Ir in the octahedral or tetrahedral environment. In this work we report the rare occurrence of square planar iridate $Cs_2Na_2IrO_4$. The structure consists of isolated IrO_4 planes, orthogonally oriented in consecutive layers. Our work involves the detailed study of electronic and magnetic properties of $Cs_2Na_2IrO_4$, from first principles calculations. Microscopic magnetic exchange interactions and Wannier function analysis reveals the quasi two dimensional canted AFM ground state, despite the absence of long range structural connectivity which originates because of very weak spin-phonon coupling. Further, the origin of orthogonally placed IrO_4 moieties can be understood from the phonon modes analysis. Belonging to the 5*d* series, Ir is known to be substantially impacted by SOC. However due to the half-filled situation, the orbital magnetic moment is quenched in this case. Nevertheless we still obtain a large magneto-crystalline anisotropy which could be explained from the second-order perturbation theory. As a guiding tool to experimentalists, we also report preliminary work on muon active sites which is crucial in obtaining the magnetic structure of the system for future studies.

MA 4.6 Mon 10:45 EB 107

Magnetic excitations beyond the single- and double-magnons — •Hebatalla Elnaggar[1], Abhishek Nag[2], Maurits Haverkort[3], Ke-Jin Zhou[2], and Frank de Groot[4] — [1]Sorbonne University - CNRS, Paris, France — [2]Diamond Light Source, Didcot, UK — [3]Heidelberg University, Heidelberg, Germany — [4]Utrecht University, Utrecht, Netherlands

Conventional wisdom suggests that one photon that carries one unit of angular momentum ($1\hbar$) can change the spin angular momentum of a magnetic site with one unit ($\delta M_s = 1\pm\ 1\hbar$) at most following the selection rules. This implies that a two-photon process such as $2p3d$ resonant inelastic X-ray scattering (RIXS) can change the spin angular momentum of a magnetic system with a maximum of two units ($\delta M_s = \pm\ 2\hbar$). Hereinwe describe a triple-magnon excitation in α-Fe_2O_3, which contradicts this conventional wisdom that only 1- and 2-magnon excitations are possible in a resonant inelastic X-ray scattering experiment [1]. We observe an excitation at exactly three times the magnon

energy, along with additional excitations at four and five times the magnon energy, suggesting quadruple and quintuple magnons as well. Guided by theoretical calculations, we reveal how a two-photon scattering process can create exotic higher-rank magnons and the relevance of these quasiparticles for magnon-based applications.

References: 1- H. Elnaggar, et. al., Magnetic excitations beyond the single- and double-magnons, Nat. Commun. 14, 2749 (2023).

15 min. break

MA 4.7 Mon 11:15 EB 107

Large thermal Hall effect in the ordered phase of $EuTiO_3$ — •Rohit Sharma, Johannes Engelmayer, Lara Pätzold, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany

We present the observation of a large thermal Hall effect in the quantum paraelectric compound $EuTiO_3$. Additionally, in $EuTiO_3$ the magnetic moments of Eu^{2+} order antiferromagnetically in a G-type configuration at $T_N \approx 5.5$ K [1]. A magnetic field of ≈ 1.5T is already sufficient to change from antiferromagnetic to polarized ferromagnetic state. We have observed a glasslike longitudinal thermal conductivity (κ_{xx}) in this material, which can be attributed to spin lattice coupling [2]. Temperature dependence of transverse thermal Hall conductivity (κ_{xy}) looks similar to κ_{xx} in the paramagnetic regime. Field dependence of κ_{xy} shows linear behaviour with a positive sign in the paramagnetic regime, but becomes very large with a highly non-monotonic when measured in the ordered phase. It shows a large negative signal in the low field range which changes sign to a small positive signal for high field values. The positive signal at higher field values can be scaled well with the magnetization data measured at same temperature. The origin of the large negative signal is not clear and possible reasons for the its occurrence in $EuTiO_3$ will be discussed.

Funded by the DFG via Project No. LO 818/6-1.
[1] J. Engelmayer et al. Phys. Rev. Mater. 3, 051401(R) (2019)
[2] A. Jaoui et al. Phys. Rev. Mater. 7, 094604 (2023)

MA 4.8 Mon 11:30 EB 107

Janh-Teller bipolarons in the spin-orbit multipolar magnetic oxide Ba_2NaOsO_6 — •Lorenzo Celiberti[1] and Cesare Franchini[1,2] — [1]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Vienna, Austria — [2]Department of Physics and Astronomy 'Augusto Righi', University of Bologna, Bologna, Italy

Complex oxides hosting 5d electrons present a variety of exotic phases arising from spin-orbital (SO) interactions and electronic correlation (EC). In the Mott insulator Ba_2NaOsO_6 (BNOO), a canted antiferromagnet with multipolar interactions, strong EC together with Jahn-Teller lattice activity pave the way for bridging polarons and SO coupling, distinct quantum effects that play a critical role in charge transport and spin-orbitronics. Polarons are quasiparticles originating from strong electron-phonon interaction and are ubiquitous in polarizable materials, especially in 3d transition metal oxides. Despite the more spatially delocalized nature of 5d electrons, we demonstrate the formation of *Jahn-Teller spin-orbital bipolarons* in electron doped BNOO by combining ab-initio calculations with nuclear magnetic resonance and muon spin rotation measurements. The polaronic charge trapping process converts the Os $5d^1$ spin-orbital $J_{eff} = 3/2$ levels, characteristic of pristine BNOO, into a $5d^2$ $J_{eff} = 2$ manifold, leading to the coexistence of different J-effective states in a single-phase material. Moreover, we suggest that polaron formation creates robust in-gap states that prevent the transition to a metal phase even at ultrahigh doping, thus preserving the Mott gap across the entire doping range.

MA 4.9 Mon 11:45 EB 107

Multipolar interactions as the origin of excitation gap in d^3 spin-orbit double perovskites — •Leonid Pourovskii — CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — Collège de France, Université PSL, 11 pl. Marcelin Berthelot, 75005 Paris, France

In Mott insulators with a half-filled t_{2g} shell the Hund's rule coupling J_H induces a spin S=3/2 orbital-singlet ground state. The spin-orbit interaction is not effective within this ground state and conventional spin orders are expected. This is the case in d^3 cubic double perovskites (DP) of heavy transition metals. However, their inelastic neutron scattering (INS) spectra feature unexpectedly large gaps. Even in the cubic DP $Ba_2YB'O_6$ (B'=Os, Ru), where single-ion anisotropy is expected to be negligible, the measured gaps are remarkably large. We employ an ab initio many-body force-theorem method to obtain effective magnetic Hamiltonians for these two systems. The calculated Hamiltonains feature unexpectedly significant multipolar - dipole-octupolar (DO) - intersite exchange interactions. The DO terms break continuous symmetry of the S=3/2 Heisenberg terms opening an excitation gap. The theoretical gap magnitudes and calculated INS spectra agree with experiment. The DO intersite coupling arises due to excited states of the t_{2g}^3 manifold admixed by spin-orbit into the $S = 3/2$ ground state. Their large relative magnitude stems from a characteristic anisotropy of t_{2g} hopping terms in DPs and scales as a square of the ratio of spin-orbit coupling and J_H.

MA 4.10 Mon 12:00 EB 107

Magnetic and lattice properties of KEr(MoO4)2 in magnetic fields up to 50 tesla — •D. Kamenskyi[1], L. Prodan[1], K. Kutko[2], V. Khrustalyov[2], S. Khmelevskyi[3], L. Pourovskii[4], B. Bernath[5], and Y. Skourski[6] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg — [2]B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Kharkiv, Ukraine — [3]Research Center for Materials Science and Engineering, Vienna University of Technology, Austria — [4]CPHT, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, France — [5]HFML-EMFL, Radboud University, Nijmegen, The Netherlands — [6]HLD-EMFL, Helmholtz-Zentrum Dresden-Rossendorf, Germany

We report a magnetisation and magnetosriction study of the rare-earth-based paramagnet KEr(MoO4)2 in magnetic fields up to 50 T. Recent observation of massive magnetostriction and rotational magnetocaloric effects triggered the interest to study the microscopic mechanism behind this phenomena. We combine several experimental techniques to investigate the magnetisation behaviour until saturation. The synergy of magnetic torque measurements and vibrating sample magnetometry allowed us to reconstruct parallel and perpendicular magnetisation, enabling us to trace its evolution up to 30 T. Our experiments reveal the saturation along all principle axes is well below the value expected from crystal electric field calculations. We argue that an applied magnetic field distorts the local environment of Er3+ ions and affects its crystal electric field splitting.

MA 4.11 Mon 12:15 EB 107

Tuning the physical properties of La0.7Sr0.3MnO(3-δ) via oxygen off-stoichiometry using assisted thermal vacuum annealing — •Chenyang Yin[1,2], Lei Cao[2], Suqin He[3,2], Tomas Duchon[4], Yunxia Zhou[5], Denis Sheptyakov[6], Maria Teresa Fernandez-Diaz[7], Shibabrata Nandi[2], and Oleg Petracic[2,1] — [1]Heinrich Heine University Düsseldorf, Faculty of Mathematics and Natural Sciences, Düsseldorf, Germany — [2]Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany — [3]Peter Grünberg Institut (PGI-7), JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany — [4]Peter Grünberg Institut (PGI-6), JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany — [5]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [6]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [7]Institut Laue-Langevin (ILL), Grenoble, France

In La0.7Sr0.3MnO(3-δ) (LSMO), the topotactic phase transition from the Perovskite (PV) phase to the layered oxygen-vacancy-ordered Brownmillerite (BM) phase can be triggered by deoxygenation. We realized this phase transition in both a strained LSMO thin film system and bulk-like unstrained LSMO powder system via assisted thermal vacuum annealing. For thin film, A metal-to-insulator and simultaneously a ferromagnetic-to-antiferromagnetic transition is found. For powder, the evolution of crystal and spin structure at different oxygen-deficient states from PV to BM is determined using neutron diffraction.