MA 42: Magnetic Heuslers, Half-Metals and Oxides (jointly with TT)

Time: Thursday 9:30–12:30 Location: H34

MA 42.1 Thu 9:30 H34

Singular manifestation of square-planar geometry and novel S=$\frac{3}{2}$ state of a iridate Na_4IrO_4 — •Sudipta Kanungo[1], Binghai Yan[1,2], Patrick Merz[1], Claudia Felser[1], and Martin Jansen[3] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187, Dresden, Germany — [3]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Local environments and valence electron counts primarily determine the electronic states and physical properties of transition metal complexes. For example, square-planar surroundings found in transition oxometalates such as cuprates, Nickaltes are usually associated with the d^8 or d^9 electron configuration. In this work, we address an experimentally observed exotic square-planar mono-oxoanion $[IrO_4]^{4-}$ in Na_4IrO_4 with Ir(IV) in d^5 (S=$\frac{3}{2}$ state) configuration, using ab-initio calculations. On contrary, in its 3d counterpart, Na_4CoO_4, Co(IV) is in tetrahedral coordination with S=$\frac{5}{2}$ high spin state. Our ab-initio calculations reveal that the on-site Coulomb interaction U is the essential factor for determining the stability of the local coordination as well as spin state. We find that due to weak Coulomb repulsion of Ir-5d electrons, Na_4IrO_4 form in a square-planar coordination whereas for Na_4CoO_4, Co(IV) is in tetrahedral coordination, due to strong electron correlation at 3d Co site. Following the trend from 5d to 3d, we predict that the intermediate 4d material Na_4RhO_4, if synthesized, may favor tetrahedral coordination but with an S=$\frac{1}{2}$ low spin state.

MA 42.2 Thu 9:45 H34

Influence of extended crystal defects on magnetic moments and magnetocrystalline anisotropy in the Heusler phase Fe_2CoGa — •Georg Krugel, Wolfgang Körner, Daniel F. Urban und Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

In the search for new and cheap rare-earth-free hard-magnetic materials, Heusler phases are promising candidates. Depending on their chemical composition, high Curie temperatures and high magnetizations without rare earth elements can be achieved. By using a computational screening approach, Gillesen et al. [1] identified several Heusler phases with high magnetic moments like Fe_2CoGa or Fe_2CoAl.

However, in order to have a good hard-magnetic material with a defined easy axis a substantial intrinsic crystalline anisotropy is needed. Unfortunately, the Heusler phases with high magnetic moment generally crystallize in the regular or inverse cubic structure with zero anisotropy. Nevertheless, extended crystal defects like stacking faults or grain boundaries may lead to preferred crystal orientations and provide a way for optimizing the magnetic anisotropy through microstructure engineering.

We present a density functional theory study on extended defects in Fe_2CoGa which illustrates how much magnetocrystalline anisotropy can be achieved. Furthermore, the impact of the extended defects on the local magnetic moments and the total magnetization is analyzed.

[1] M. Gillessen and R. Dronskowski, J. Comput. Chem. 30, 1290 (2009)

MA 42.3 Thu 10:00 H34

Introducing magnetic functionality into oxide heterostructures by thermodynamic stabilization: $EuO/SrTiO_3$ — •Patrick Lömker[1], Timm Gerber[1], Andrei Gloskovskii[2], Wolfgang Drube[2], and Martina Müller[1,3] — [1]Forschungszentrum Jülich GmbH, PGI-6, Jülich, Germany — [2]DESY Photon Science, DESY, Hamburg, Germany — [3]Universität Duisburg-Essen, Duisburg, Germany

In order to introduce magnetic functionality into all-oxide heterostructures, we integrated ultra thin films of the ferromagnetic insulator EuO epitaxially on conducting 0.5% Nb doped $SrTiO_3$(001) (Nb:STO).

We circumvented the use of thick buffer layers (e.g. SrO) to prevent over-oxidation of EuO films by making use of the thermodynamic properties of Eu metal to ultimately form EuO. In particular, *in situ* XPS shows that Eu-metal only deposition on Nb:STO leads to the formation of ultrathin stoichiometric EuO films through substrate supplied oxygen. Furthermore, the interplay between oxygen pressure, Eu flux and T_S is utilized to extended stoichiometric growth to larger film thicknesses. For $T_S = 20°C$ we report the formation of fully stoichiometric EuO films, whereas growth at elevated temperature (250-500°C) yields epitaxial integration with sub-ML interfacial Eu_2O_3.

Further analysis by LEED, RHEED and XRD reveals the epitaxial relationship EuO(110)/Nb:STO(100). *Ex situ* magnetic analysis shows bulk-like properties for optimized EuO ultra thin films. Finally, HAXPES experiments were performed at PETRA III confirming the thermodynamical stabilization of ferromagnetic EuO on Nb:STO.

MA 42.4 Thu 10:15 H34

Exchange Bias-Like Effect of an Uncompensated Antiferromagnet — •Bastian Henne, Verena Ney, Mariano de Souza, and Andreas Ney — Johannes Kepler Universität Linz - Austria

Commonly, exchange biasing is evidenced by a field-like *horizontal* shift of the $M(H)$-loop dominated by the FM [1]. In contrast, its microscopic origin is attributed to uncompensated spins, *i.e.*, an excess magnetization, of the antiferromagnet (AFM) exchange coupled to the FM [2]. This infers the presence of an additional *vertical* shift . Experimental observations of this shift are limited to few layered FM/AFM systems (for example [3]) and observations in the absence of a FM are lacking. In this contribution we present antiferromagnetic Co:ZnO as model system in which the uncompensated spins indeed exclusively lead to a vertical shift which is measurable by conventional magnetometry. Our findings pave the way for the exploration of the vertical exchange bias effect in the absence of a FM and the possibility to achieve a finite field-resistant magnetization in an uncompensated AFM.

[1] Nogúes, J. and Schuller, I.K., J. Magn. Magn. Mater. **192**, 203 (1999).

[2] Ohldag, H. *et al.*, Phys. Rev. Lett. **91**, 017203 (2003).

[3] Rana, R. *et al.*, Sci. Rep. **4**, 4138 (2014).

MA 42.5 Thu 10:30 H34

Magnetic properties of Fe doped spinel $CoCr_2O_4$ studied from first principles theory — •Biplab Sanyal, Shreemoyee Ganguly, and Raghuveer Chimata — Department of Physics and Astronomy, Uppsala University, Box-516, 75120 Uppsala, Sweden

We present a systematic study of the effects of Fe doping on the electronic and magnetic structures of spinel $CoCr_2O_4$ by ab initio density functional theory and Monte Carlo simulations. Our calculated magnetic structure for pristine $CoCr_2O_4$ correctly reproduces the experimental one with a q-vector of (0.67, 0.67,0.0). We show that the non-collinear spin structure with a non-zero q-vector in the spinel structure is driven towards collinearity by Fe doping by a complex interplay between interatomic exchange interactions. In the inverse spinel structure with 100 % Fe doping, a collinear antiferromagnetic order develops along with a half metallic electronic structure, which evolves due to the chemical disorder between Fe and Co in the B sites described by the coherent potential approximation. To the best of our knowledge, this is the first comprehensive theoretical study to understand the evolution of magnetic and electronic properties of multiferroic $CoCr_2O_4$ doped with Fe.

15 min. break

MA 42.6 Thu 11:00 H34

Thermodynamic Stability and Control of Oxygen Reactivity at Magnetic Oxide Interfaces: EuO on ITO — •Timm Gerber[1], Patrick Lömker[1], Bernardus Zijlstra[1], Claire Besson[2], David Müller[1], Willi Zander[3], Jürgen Schubert[3], Mihaela Gorgoi[4], and Martina Müller[1,5] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Jülich, Germany — [2]Institut für Anorganische Chemie, RWTH Aachen University, Germany — [3]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, Jülich, Germany — [4]Helmholtz-Zentrum für Materalien und Energie GmbH, Berlin, Germany — [5]Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany

As a prototypical all-oxide heterostructure, the ferromagnetic insulator europium monoxide (EuO) is synthesized on transparent and conductive indium tin oxide (ITO) virtual substrates. Non-destructive hard X-ray photoelectron spectroscopy (HAXPES) is employed to depth profile the chemical composition of the magnetic layer and the buried oxide-oxide interface. We find that the otherwise well-established

adsorption-controlled EuO growth mode is not applicable here due to thermally activated oxygen diffusion from ITO. We present how to control the oxygen reactivity at the interface and discuss its origin in a thermodynamic analysis. Our complementary methodical strategy allows for a significant improvement of ultrathin EuO films with sizeable magnetic properties. Generally, our approach derives guidelines for the proper choice of oxide substrates and buffer layer materials for functional all-oxide heterostructures.

MA 42.7 Thu 11:15 H34

Ti_2MnZ (Z=Al, Ga, In) compounds: Nearly spin gapless Semiconductors — •Hongying Jia[1,2], Xuefang Dai[2], and Guodong Liu[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]School of Material Sciences and Engineering, Hebei University of Technology, Tianjin 300130, P. R. China

Spin gapless semiconductors with-low spin magnetic moments are promising functional materials due to their fascinating potential for realistic applications. The ideal spin gapless semiconductors exhibit zero magnetic moment and low external magnetic fields, leading to smaller energy losses. However, spin gapless semiconductors with zero magnetic moments are rarely reported up to now. Therefore, it is necessary to clarify the differences in the origin of the band gap in two spin channels for spin gapless magnetic semiconductors with Heusler structure. In our work [1], the electronic, structural and magnetic properties of Ti_2MnZ (Z=Al, Ga, In) compounds were systematically investigated using first-principles calculations. Our results demonstrate that these compounds are nearly spin gapless semiconductors and have a zero magnetic moment. The origin of the band gap in different spin directions will be discussed in detail. Besides, the effects of the lattice parameter and doping effects of the congeners on the width of the band gaps are demonstrated. These results will help to better understand the mechanism of spin gapless semiconductors and therefore promote the design of new spin gapless semiconductors.

[1] H. Y. Jia *et al.*, AIP Advances **4**, 047113 (2014)

MA 42.8 Thu 11:30 H34

Contributions from conduction electrons and localized moments to the magnetization in Cu_2MnAl as separated by spin polarized measurements — •Josef Andreas Weber[1], Andreas Bauer[1], Peter Böni[1], Hubert Ceeh[1], Stephen Dugdale[2], Atsuo Kawasuso[4], Michael Leitner[3], Christian Pfleiderer[1], and Christoph Hugenschmidt[1,3] — [1]Physik-Department, Technische Universität München, James-Franck Straße, 85748 Garching, Germany — [2]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK — [3]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [4]Advanced Science Research Center, Japan Atomic Energy Agency, 1233 Watanuki, Takasaki, Gunma 370-1292, Japan

The distinction between localized and itinerant ferromagnetism is for some systems still a contentious issue. In Mn based Heusler systems it is usually assumed, that all the magnetic moments are localized at the Mn atoms. However it was shown, that in Cu_2MnAl there exist different Fermi surfaces for the majority and minority spin channel and therefore also the conduction electrons contribute substantially to the the total magnetic moment [1]. Here we report our results obtained by comparing spin polarized 2D-ACAR measurements with recent magnetic Compton scattering measurements and with spin polarized positron lifetime experiments.

[1] J. A. Weber et al., Phys. Rev. Lett. **115** 206404 (2015).

MA 42.9 Thu 11:45 H34

Chemical disorder as engineering tool for magnetic properties and spin-polarization in Mn3Ga-based Heusler systems — •Lukas Wollmann, Stanislav Chadov, Sunil Wilfred D'Souza, Gerhard H. Fecher, and Claudia Felser — Max-Planck-Insitute for Chemical Physics of Solids

The present contribution discusses the effect of random substitution of Mn in Mn_3Ga as a constructive disorder phenomenon, which, for instance, allows to chemically control the spin-polarization of the charge carriers. It is based on *spin-selective electron localization* encountered by the first-principles calculations on the family of tetragonal Mn-based Heusler materials $Mn_{3-x}Y_xGa$ [1,2]. Our calculations indicate that *spin-selective localization* can be introduced by substituting Mn with almost any 3d transition metal element (Sc, Ti, V, Cr, Fe, Co, Ni, Cu) as well as with several heavier species as Os, Ir or Pt. The spin-polarization was derived from the spin-projected residual conductivity tensor computed within the Kubo-Greenwood formalism within the SPR-KKR method [3], which properly accounts for the effects of electron localization induced by the scattering due to chemical disorder. In this way one might obtain the series of highly spin-polarized alloys with noticeable magnetocrystalline anisotropy, combining the advantages of tetragonal and cubic Heusler compounds.

[1] S. Chadov *et al.*, Phys. Rev. B **91** 094203 (2015); [2] L. Wollmann *et al.*, J. Phys. D: Appl. Phys. **48** 164004 (2015); [3] H. Ebert *et al.*, Rep. Prog. Phys. **74** 096501 (2011).

MA 42.10 Thu 12:00 H34

Yttrium Iron Garnet Thin Films with Very Low Damping Obtained by Recrystallization of Amorphous Material — •Christoph Hauser[1], Tim Richter[1], Nico Homonnay[1], Christian Eisenschmidt[1], Hakan Deniz[2], Dietrich Hesse[2], Stefan Ebbinghaus[1], and Georg Schmidt[1] — [1]Martin-Luther University Halle-Wittenberg, Halle, 06120, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, 06120, Germany

Yttrium Iron Garnet is a room temperature ferrimagnet, which has recently gained importance for magnonics [1]. For the integration into magnonic devices, however very thin films must be used which are mostly fabricated by pulsed laser deposition (PLD) and often suffer from increased damping. Using room temperature deposition and subsequent annealing in an oxygen atmosphere much lower damping can be achieved. For a 56 nm thick layer a damping constant of $\alpha = 6.15 \cdot 10^{-5}$ and a linewidth as small as 1.30 Oe @9.6 GHz are obtained which are the lowest values for PLD grown thin films reported so far. Even for a 20 nm thick layer a damping constant of $\alpha = 7.39 \cdot 10^{-5}$ is found. In this case the FMR linewidth is 3.49 Oe @9.6GHz. The layers show high crystalline quality and sub nanometer surface roughness in various structural characterizations. Our results not only present a method of depositing thin film YIG of unprecedented quality but also open up new options for the fabrication of thin film complex oxides or even other crystalline materials. We are going to present the results of various experiments using different layer thicknesses and annealing parameters. [1]Chumak et al. Nat. Commun. 5, 4700 (2014).

MA 42.11 Thu 12:15 H34

Competing Superexchange Interactions in Sr2-xCaxCoOsO6 Double Perovskite Osmates — •Ryan Morrow[1,2], Rohan Mishra[1], Oscar D. Restrepo[1], Molly R. Ball[1], Wolfgang Windl[1], Sabine Wurmehl[2,3], Ulrike Stockert[2,3], Bernd Büchner[2,3], Jiaqiang Yan[4], Michael A. McGuire[4], John W. Freeland[5], Daniel Haskel[5], and Patrick M. Woodward[1] — [1]OSU, Columbus, OH, United States — [2]IFW, Dresden, Germany — [3]TUD, Dresden, Germany — [4]ORNL, Oak Ridge, TN, United States — [5]ANL, Argonne, IL, United States

Double perovskites containing mixed transition metal cations have exhibited numerous desirable properties such as colossal magnetoresistance, half metallic transport, and high temperature ferrimagnetism. However, a predictive understanding of the superexchange mechanisms which control the magnetism of these materials when they are insulating and contained ordered 3d and 4d or 5d transition metals has remained elusive. In this work, the novel insulators Sr2CoOsO6, SrCaCoOsO6, and Ca2CoOsO6 are studied through a combination of AC and DC magnetometry, specific heat, X-ray magnetic circular dichroism, and neutron powder diffraction in order to characterize two antiferromagnetic orders in Sr2CoOsO6, two spin glass transitions in SrCaCoOsO6, and ferrimagnetic ordering in Ca2CoOsO6. The details of the crystal structures will be used to draw connections between the tuning of bonding geometry through chemical pressure and the competition between short and long range superexchange interactions on the resulting magnetic ground states.