TT 23: Magnetic Heuslers, Half-Metals, Semiconductors, and Oxides (organized by MA)

Time: Monday 15:00–18:45 Location: H 1012

TT 23.1 Mon 15:00 H 1012

The role of spin-orbit coupling and complex magnetism in the electronic structure of bulk and thin film $CaIrO_3$ — •Kerstin Dörr, Yuriy Mokrousov, Stefan Blügel, and Marjana Lezaic — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

One of the very lively research fields in condensed-matter physics is focussing on transition-metal oxides (TMO), due to a large variety of interesting physical properties they present that can be exploited in potential applications. Especially the question what drives a TMO to become insulating or metallic is an ongoing discussion, owing to the complexity of the physical effects that play a role in such systems. E.g., in well studied 3*d* compounds the enhanced onsite Coulomb repulsion drives the system into an insulating state. In contrast to this, in 5*d* TMOs the Coulomb repulsion is reduced but its interplay with the spin-orbit coupling can again force the system to become insulating, undergoing the so called spin-orbital Mott transition. In this talk we will discuss these effects in the 5*d* TMO $CaIrO_3$ in orthorhombic perovskite form. Furthermore, we will present our first-principles study of the influence of magnetism and the modifications of the bulk bandstructure of this compound in thin films.

TT 23.2 Mon 15:15 H 1012

Anisotropy of magnetic interactions in β-Li_2IrO_3 — •Alexander Yaresko and Yoshiro Nohara — MPI FKF, Stuttgart, Germany

Iridium oxides α-Li_2IrO_3 and α-Na_2IrO_3 with a honeycomb lattice attracted much attention as possible candidates for realization of a Kitaev model with bond-dependent anisotropic magnetic interactions. Recently, another complex Ir oxide β-Li_2IrO_3 has been synthesized which is expected to be close to forming a Kitaev spin liquid. Ir ions in this oxide form a "hyper-honeycomb" lattice, a three-dimensional analogue of the honeycomb lattice of α-Na_2IrO_3. We performed LDA+U band structure calculations for β-Li_2IrO_3 with different magnetic orderings of Ir magnetic moments. The results are mapped onto a model which includes isotropic Heisenberg-like as well as bond-dependent anisotropic interactions. It is shown that the contribution of the anisotropic interactions to the magnetic energy is at least as strong as isotropic one.

TT 23.3 Mon 15:30 H 1012

Kitaev interactions in $4d_5$ honeycomb systems: Li_2RhO_3 vs $RuCl_3$ — •Ravi Yadav, Vamshi Mohan Katukuri, Satoshi Nishimoto, Liviu Hozoi, and Jeroen Van Den Brink — Institute forTheoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany

While electronic-structure calculations within either the wavefunction-based [1,2] or density functional theory [3] framework agree on the magnitude and the signs of the Kitaev couplings in $5d^5$ honeycomb iridates, much less is known on these effective exchange constants in the $4d^5$ analogues. We here discuss the outcome of many-body, wavefunction-based quantum chemistry computations for these interaction parameters in Li_2RhO_3 and $RuCl_3$. The ab initio values for the nearest-neighbor couplings, both isotropic and anisotropic, are further fed to an extended spin Hamiltonian that includes additionally 2^{nd}- plus 3^{rd}-neighbor Heisenberg terms and on the basis of exact-diagonalization calculations predictions are made for the nature of the magnetic ground states in these compounds.

[1] Vamshi M. Katukuri et al, New J. Phys. 16 (2014) 013056.
[2] Satoshi Nishimoto et al, arXiv:1403.6698.
[3] Youhei Yamaji et al, Phys. Rev. Lett. 113, 107201.

TT 23.4 Mon 15:45 H 1012

Magnetic excitations in the anomalous ferromagnetic metal $SrRuO_3$ — •Stefan Kunkemöller[1], A. Agung Nugroho[2], Yvan Sidis[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937, Germany — [2]Faculty of Mathematics and Natural Sciences, Jl. Ganesa 10 Bandung, 40132, Indonesia — [3]Laboratoire Léon Brillouin, CEA Saclay, F-91191 Gif sur Yvette Cedex, France

$SrRuO_3$ is the infinite-layer perovskite of the Ruddlesden-Popper series of ruthenates. It exhibits ferromagnetic ordering and highly anomalous electronic properties. At Cologne University we could recently grow several $SrRuO_3$ single-crystals with a mass of few grams each using a Canon Machinery image furnace. Inelastic neutron scattering experiments on the magnon dispersion were performed at the 2T thermal triple-axis spectrometer of the Laboratoire Léon Brillouin in Saclay. At intermediate energies and low temperature an isotropic magnon dispersion is observed as it is expected for a nearly cubic material. The magnon dispersion along the three main-symmetry directions of the pseudo-cubic material can be described by simple spin-wave theory with a gap of 1.7(2) meV and a magnetic stiffness constant of 95(5) meVÅ^2. Strong magnon-like scattering is observed till 280 K and there is no evidence for essential softening of the dispersion across the magnetic ordering in contrast to any simple Heisenberg model.

TT 23.5 Mon 16:00 H 1012

Induced magnetic monopoles on magnetoelectric surfaces — •Quintin Meier, Michael Fechner, and Nicola A. Spaldin — ETH Zürich, Department for Materials, Zürich, Switzerland

We calculate the magnetic fields caused by a point charge adjacent to the surface of a magnetoelectric, that is a material in which an electric field induces a magnetization and vice versa. The electric point charge induces monopolar and quadrupolar magnetic fields in the magnetoelectric[1]. However in the outside area the field is purely monopolar ($B \propto r^{-2}$). We show that this behaviour is valid not only for materials with isotropic magnetoelectric responses[2], but for the broader class of uniaxial magnetoelectric materials as well. Moreover, our analysis of the field strength shows that a already single charge near the prototypical uniaxial magnetoelectric, Cr_2O_3, induces a monopolar stray field which should be detectable by experiment. [1] Fechner, M. et al., Phys. Rev. B. 89, 184415 (2014) [2] Qi, X.-L. et al., Science, 323(5), 1184 (2009)

TT 23.6 Mon 16:15 H 1012

Ab initio study of the magnetic properties of Sr_2FeMoO_6 with defects — •Martin Hoffmann[1,2], Victor N. Antonov[3], Wolfram Hergert[1], Arthur Ernst[2,4], and Lev Bekenov[3] — [1]Martin Luther University Halle Wittenberg, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Institute for Metal Physics, Kiev, Ukraine — [4]University Leipzig, Germany

We used first-principle calculations with the Korringa-Kohn-Rostoker Green function method to systematically investigate the electronic and magnetic properties of Sr_2FeMoO_6 (SFMO). We applied self-interaction correction and GGA+U to take into account the correlation effects and obtain the half-metallic nature of the material. The Curie temperature T_C was obtained from calculated magnetic exchange interactions which were used in a Monte Carlo simulation.

For a continuously increasing U parameter, SFMO became half-metallic but the T_C decreased below the reported values for bulk SFMO. We investigated possibilities to find a better agreement with experiment. This might be shortcomings in the description of the electronic structure, changes in the valency of Fe or the appearance of defects like antisite disorder and oxygen vacancies.

In addition, x-ray absorption spectra were simulated with the linear muffin-tin orbital method and compared to experimental results. A good agreement was only obtained by considering a contribution of Fe^{2+} and oxygen vacancies.

TT 23.7 Mon 16:30 H 1012

Electrical and magnetic characterization of electrospun $La_{1-x}Sr_xMnO_3$ nanowires — •Thomas Karwoth[1], Xian Lin Zeng[1], Andrew Kostrubanic[2], Michael Koblischka[1], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, P.O.Box 151150, D-66041 Saarbrücken, Germany — [2]Drexel University, Philadelphia, Pennsylvania 19104, USA

Nanowires of the material class $La_{1-x}Sr_xMnO_3$ with different doping levels x = 0.2, 0.33, 0.5 were fabricated employing a sol-gel-process via electrospinning and a subsequent thermal treatment process based on thermal gravity analysis results. Investigations by means of scanning electron microscopy revealed an average diameter of the resulting nanowires of around 220 nm and a length of more than 50 μm. The chemical phases of the samples have been confirmed via X-Ray diffrac-

tion. The nanowires are polycrystalline with a grain size of about 15-17 nm, which corresponds to the result obtained from transmission electron microscopy. Analyses of the electronic transportation properties and of the magnetoresistive effects of the nanowire samples were carried out by a four probe measurement inside a bath cryostat. Of interest are size effects and the dependence of the properties on the stoichiometry. SQUID measurements of $M(T)$ and $M(H)$ at room temperature, 77 K and 4.2 K were carried out as well, revealing the soft magnetic character of the nanowires.

TT 23.8 Mon 16:45 H 1012

High quality Yttrium Iron Garnet grown by room temperature pulsed laser deposition and subsequent annealing — •Christoph Hauser[1], Tim Richter[1], Nico Homonnay[1], Bodo Fuhrmann[2], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale) , Germany

Yttrium Iron Garnet is a room temperature ferrimagnet, which has recently gained importance due to its application in spin pumping and the investigation of the inverse spin Hall effect [1]. The linewidth and damping which can be observed in ferromagnetic resonance are typically the most important quality criteria for YIG films. Ultrathin films with very low damping constants can been grown by pulsed laser deposition [2]. We have investigated different methods of PLD growth to obtain high quality YIG thin films. Using PLD at high substrate temperature, 20 nm thick YIG films with a FMR linewidth of 12 Oe at 9.6 GHz could be obtained. Even better quality is achieved when the YIG is deposited at room temperature and subsequently annealed in an oxygen atmosphere, where we can obtain a linewidth of less than 2 Oe at 9.6 GHz. The layers show high crystalline quality and subnanometer surface roughness in X-ray diffraction and reflectometry. We are going to present the results of various experiments using different layer thicknesses and annealing parameters. [1]K. Uchida et al., Appl. Phys. Lett. 97, 252504 (2010) [2]d'Allivy et al., Appl. Phys. Lett. 103, 82408 (2013)

15 min. break

TT 23.9 Mon 17:15 H 1012

Magnetostriction in pulsed magnetic fields up to 70 T - the spin states in $LaCoO_3$ — •Mathias Doerr[1], Martin Rotter[2], Sergey Granovsky[1], Michael Loewenhaupt[1], and Zhaosheng S. Wang[3] — [1]TU Dresden, Institut für Festkörperphysik, D-01062 Dresden — [2]MPI for Chemical Physics of Solids, D-01187 Dresden — [3]FZ Dresden-Rossendorf, Hochfeld-Magnetlabor, D-01314 Dresden

Magnetoelastic investigations in pulsed magnetic fields with a pulse duration of about 10 ms are still challenging. The new optical FBG method overcomes the difficulty of mechanical noise and offers a resolution in the order of 10^{-6}. As an example, the spin states in $LaCoO_3$, important for understanding of spin-dependent transport in oxides, were analyzed by longitudinal and transversal magnetostriction measurements up to 70 T. The data show a sharp magnetic transition at about 60 T accompanied by a large volume, but only small distortion effect. Supplemented by electronic energy calculations this confirms a correlated low-to-high spin (LS/HS) transition in contrast to the propagated intermediate spin-state scenario (LS-IS-HS).

TT 23.10 Mon 17:30 H 1012

Magnetic properties of the double perovskite Sr2FeOsO6: microscopic insights from ab-initio density-functional theory study — •sudipta kanungo[1], binghai yan[1,2], martin jansen[3], and claudia felser[1] — [1]Max-Planck-Institut fur Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Max-Planck-Institut fur Physik komplexer Systeme, 01187, Dresden, Germany — [3]Max-Planck-Institut fur Festkorperforschung, 70569 Stuttgart, Germany

Using density-functional theory calculations, we investigated the electronic and magnetic properties of the ordered 3d-5d double perovskite Sr2FeOsO6, which has recently drawn attention for interesting two step antiferromagnetic (AFM) phase transitions at low temperature in experiments. The calculated effective magnetic exchange interactions reveal the importance of long-range super-super-exchange interactions in this compound. The competition between the weak ferromagnetic Os-O-Fe short-range interaction and strong AFM Os-O-Fe-O-Os long-range interaction induces strong magnetic frustration along the crystallographic c axis. This frustration is proposed to drive the magnetic phase transition between two AFM phases in the low temperature and related lattice distortion, which were observed in experiment.

[Ref: Sudipta Kanungo, Binghai Yan, Martin Jansen, and Claudia Felser; Phys. Rev. B 89,214414 (2014)]

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TT 23.11 Mon 17:45 H 1012

Structure and magnetic interactions in Ba3-xSrxCr2O8 — •Alsu Gazizulina, Henrik Grundmann, and Andreas Schilling — Physik-Institut of University of Zurich, Zurich, Switzerland

The spin dimer systems Ba3Cr2O8 and Sr3Cr2O8 are two candidates for the Bose Einstein condensation (BEC) of magnetic quasiparticles (triplons). We have recently reported on a peculiar non-linear tuning of the magnetic interaction constant J0 in the corresponding solid solution Ba3-xSrxCr2O8 by varying the Sr content x. By performing theoretical calculations based on the crystal structure, we could well reproduce the observed variation in J0. As the critical field Hc of the triplon BEC strongly depends on the magnetic interactions in the system, we have also probed the dependency of this critical field on x. Here, we report on the observed relationship between J0(x) and Hc(x) in Ba3-xSrxCr2O8.

TT 23.12 Mon 18:00 H 1012

Investigation Of Crystal Structure, Magnetic And Transport Properties Of La2Ni(1-X)Mn(1+X)O6 (X= -0.2; 0; 0.2; 0.4; 0.6; 0.8; 1.0) — •Gizem Aslan Cansever[1,3], Franziska Scheibel[2], Mehmet Acet[2], Ergun Tasarkuyu[1], and Michael Farle[2] — [1]Mugla Sitki Kocman University, Science Faculty,48000 Mugla, Turkey — [2]Faculty of Physics, University of Duisburg-Essen, D-47057 Duisburg — [3]IFW Dresden, Institute for Solid State Research, D-01069 Dresden, Germany

La2NiMnO6 double perovskit materials show semiconductor and ferromagnetic properties which are important in terms of spintronics applications. In this study, La2Ni(1-x)Mn(1+x)O6 materials were investigated in relation to structural, electrical and magnetic properties with varying Ni and Mn concentrations. The compounds were prepared by using the sol-gel method and then heat treated in a cylindrical furnace at 1000 °C for 24 hours. The energy dispersive x-rays (EDX) analysis shows that the actual compositions of the compounds are very close to the targeted compositions and no impurity phase is present. From the analysis of x-ray diffraction data, it was observed that La2Ni1.2Mn0.8O6 and La2NiMnO6 compounds have monoclinic structure (P21/n), but the rest of the compounds exhibit the orthorhombic (Pbnm) structure. Electrical resistivity measurements show that all compunds have semiconductor behaviour. The magnetization measurements show that La2Mn2O6 incorporates both antiferromagnetic and ferromagnetic interactions. All other investigated compounds show ferromagnetic behaviour.

TT 23.13 Mon 18:15 H 1012

Neutron scattering studies of the field-induced magnetic phases of the Helimagnetic Spinel compound $ZnCr_2Se_4$. — •Alistair Cameron[1], Dmytro Inosov[1], Pavlo Portnichenko[1], Maksym Surmach[1], and Vladimir Tsurkan[2] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01069 Dresden — [2]Universität Augsburg, 16135 Augsburg

$ZnCr_2Se_4$ is a magnetoelectric compound with a cubic spinel (m3m) structure. Magnetic materials with a spinel structure present a strong opportunity to study the interplay between spin, charge and orbital degrees of freedom in a topologically frustrated environment. Particularly, those exhibiting magnetoelectric effects are of particular interest. In zero applied field, the Cr^{3+} S=3/2 moments form an incommensurate magnetic ground state with a screw structure along the (001) direction with a T_N of 20 K, which transforms into a spin spiral state in a magnetic field.

We have performed small angle neutron scattering (SANS) measurements on this spin structure for fields applied along the (100) and (110) directions. We find a field and temperature dependent structure for both field directions, with the reciprocal space propagation vector decreasing with increasing temperature and applied field, and showing a sharp jump in propagation vector across the domain selection transition. The phase diagram deduced by SANS for both field directions appear identical. In addition to investigating the AFM phase, we also probed the proposed spin nematic phase observing no SANS signal in this state, suggesting a lack of long range order.

TT 23.14 Mon 18:30 H 1012

Intrinsic resonances in the Mn spin system of ZnMnSe quantum wells — •Janina Rautert[1], Jörg Debus[1], Vitalii Yu. Ivanov[2], Sergey M. Ryabchenko[3], Andrei A. Maksimov[4], Dmitri R. Yakovlev[1,5], and Manfred Bayer[1,5] — [1]Experimentelle Physik 2, TU Dortmund, Dortmund, Germany — [2]Institute of Physics, Warsaw, Poland — [3]Institute of Physics, Kiev, Ukraine — [4]Institute of Solid State Physics, Chernogolovka, Russia — [5]Ioffe Physical-Technical Institute, St. Petersburg, Russia

Diluted magnetic semiconductors (DMS) are regarded as model structures for new types of spin electronic devices aiming at the control of the spin degree of freedom of the carriers. Although it is known that the spin-lattice interaction of the localized Mn spins is strongly accelerated by the concentration of these spins [1], a comprehensive understanding of the real mechanism of this acceleration is still missing. We observe in the stationary and time-resolved giant Zeeman energy of the exciton in ZnMnSe quantum wells a number of minima around specific magnetic fields below 10 T. These minima depend on the optical power and Mn concentration; the photoluminescence linewidth and amplitude are also affected. We propose that at these magnetic fields the levels of excited single Mn ions and quick-relaxing antiferromagnetically coupled pairs of Mn ions have anti-crossings, thus providing highly efficient magnetization relaxation. These novel results shall contribute to the understanding of spin interactions within the Mn spin system in II-VI DMS structures. [1] J. Debus et al., Phys. Rev. B 82, 085448 (2010).