MA 11: Magnetic Heuslers, Half-metals and Oxides II (with TT)

Time: Monday 15:00–18:45 Location: BEY 118

Invited Talk MA 11.1 Mon 15:00 BEY 118

Design principles of Dirac fermions and Mott insulating states in (111) oriented perovskite superlattices — •Rossitza Pentcheva — Ludwig Maximilians University, Munich, Germany

Oxide interfaces exhibit a broad spectrum of functional properties that are not available in the respective bulk compounds, such as two-dimensional conductivity, superconductivity and magnetism. With their distinct topology, (111) perovskite superlattices promise to host even more exotic electronic states compared to the much studied (001)-oriented systems. Material-specific density functional theory calculations with an on-site Coulomb repulsion term are used to explore the role of confinement, symmetry breaking, polarity mismatch and strain in the emergence of novel phases. The results illuminate a rich set of competing ground states in $(LaAlO_3)_M/(SrTiO_3)_N(111)$ [1] and $(LaNiO_3)_N/(LaAlO_3)_M(111)$ superlattices, ranging from spin-polarized, Dirac-point Fermi surfaces to charge-ordered Mott or Peierls insulating phases. Orbital reconstructions and metal-to-insulator transitions depend critically on the thickness of the quantum well N and in-plane strain, thus opening avenues for engineering properties at the nanoscale. Research in collaboration with D. Doennig and W.E. Pickett, supported by the DFG, SFB/TR80. [1] D. Doennig, W. E. Pickett, and R. Pentcheva, Phys. Rev. Lett. **111** 126804 (2013).

15 min. break

MA 11.2 Mon 15:45 BEY 118

Giant Verwey transition in magnetite thin films — Mehrdad Baghaie Yazdi and •Lambert Alff — Institut für Materialwissenschaft, TU Darmstadt

The Verwey transition in magnetite is an enigmatic challenge of solid state physics since several decades. It is generally believed that the change in magnetic moment at the Verwey transition is due to a change in magnetocrystalline anisotropy and spin reorientation. In thin films of magnetite with extraordinary high Verwey transition at 128 K, we have observed a giant change of magnetic moment above 1000%. Using several methods including neutron reflectometry we rule out spin reorientation as the origin of our observation. In addition, Raman scattering experiments show that the structural phase transition occurs at temperatures above the magnetic Verwey transition while, in contrast, newly emerging modes indicating additional charge and orbital order appear only at the Verwey transition. This result suggests that the structural phase transition in magnetite is a necessary precursor triggering a transition into a complex charge and orbitally ordered state.

MA 11.3 Mon 16:00 BEY 118

$NiFe_2O_4$: a candidate for efficient spin filtering at room temperature? — •Michael Hoppe[1], Sven Döring[1], Mihaela Gorgoi[3], Felix Gunkel[4], Claus M. Schneider[1,2], and Martina Müller[1,2] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen — [3]BESSY II, Helmholtz-Zentrum Berlin für Materialien und Energie — [4]Peter-Grünberg-Institut (PGI-7), Forschungszentrum Jülich

For the optimized performance of spintronic devices, one major challenge is to create highly spin-polarized electron currents. One promising approach is the usage of both insulating and magnetic tunnel barriers, with a highly spin-dependent tunneling probability. For this purpose, the spinel ferrite $NiFe_2O_4$ (NFO) is a very auspicious material since it shows both features even at room temperature.

To realize magnetic tunnel junctions, it is necessary to grow NFO films (d < 5 nm) which maintain quasi bulk-like properties down to this ultrathin film limit. Therefore, NFO films with varying thickness between 2 and 20 nm are deposited on Nb-doped $SrTiO_3$ substrates via pulsed laser deposition. HAXPES, XRD and XANES measurements reveal them to be chemically and structurally comparable to the bulk material. XMCD studies of the Ni- and Fe-L-edges in those films show that the alignment of the magnetic moments carried by these elements is preserved for all thicknesses. The insulating behavior is confirmed by CFM measurements. On this basis, we fabricated Nb:STO/NFO/Au tunnel junctions by means of optical lithography and characterized their electrical transport properties.

MA 11.4 Mon 16:15 BEY 118

Combined theoretical and optical band gap determination of NiFe2O4 and CoFe2O4 — •Markus Meinert and Günter Reiss — Center for Spinelectronic Materials and Devices, Bielefeld University, Germany

In a theoretical study we investigate the electronic structure and the band gap of the inverse spinel ferrites $NiFe_2O_4$ (NFO) and $CoFe_2O_4$ (CFO). The experimental optical absorption spectrum of NFO is well reproduced by fitting the Tran-Blaha parameter in the modified Becke-Johnson (mBJLDA) potential. For CFO, the agreement is less satisfying. The accuracy of the commonly applied Tauc plot to find the optical gap is assessed based on the computed spectra and we find that this approach can lead to a misinterpretation of the experimental data.

The minimum gap of $NiFe_2O_4$ is found to be a 1.53 eV wide indirect gap, which is located in the minority spin channel. In $CoFe_2O_4$, the band gap is about 0.9 eV wide and is also located in the minority spin channel.

MA 11.5 Mon 16:30 BEY 118

Exploring spin-filter tunneling in single-crystalline magnetic oxide heterostructures — •Bernardus Zijlstra[1], Patrick Lömker[1], Christian Caspers[1], Michael Hoppe[1], Jürgen Schubert[2], Willi Zander[2], Mihaela Gorgoi[3], Claus M. Schneider[1], and Martina Müller[1] — [1]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich — [3]BESSY II, Helmholtz-Zentrum Berlin

Magnetic insulators, like Europium Oxide (EuO) are of tremendous interest for spintronic research, since they can generate highly spin-polarized currents. In contrast to conventional tunneling, spin-filter tunneling through single-crystalline magnetic insulator barriers is not yet fully understood.

In order to realize fully epitaxial magnetic oxide tunnel barriers, ultrathin EuO films were grown directly on conductive Sn-doped In_2O_3 (001) (ITO), Nb-doped $SrTiO_3$ (001) (STO) and As-doped Si (001).

The EuO heteroepitaxy was characterized by LEED, RHEED and XRD, whereas the magnetic and chemical properties were analyzed by SQUID and hard x-ray photoelectron spectroscopy. We find EuO/Si(001) and EuO/STO(001) to be epitaxial, stoichiometric and to display bulk-like magnetic properties, however, EuO/ITO(001) is strongly affected by oxygen diffusion at elevated T_S. Electrical transport experiments reveal the respective spin filter tunneling properties.

MA 11.6 Mon 16:45 BEY 118

Direct observation of half metallicity in the Heusler compound Co2MnSi — •Martin Jourdan[1], Alexander Kronenberg[1], Jan Minar[2], Michaela Kolbe[1], Andrey Gloskovskij[3], Gerd Schönhense[1], Hans Joachim Elmers[1], Stanislav Chadov[4], Claudia Felser[4], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]Department Chemie und Biochemie, Ludwig-Maximilians-Universität München — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Heusler compounds are in the focus of interest due to their predicted half-metallic properties, which makes them highly interesting for spintronics. Apart from applications those materials are a test for modern band structure calculations for materials with electronic correlations of medium strength. Although a large body of those calculations is available, their experimental verification remains a major task. Here epitaxial thin films of the compound Co2MnSi are investigated in-situ by UV-photoemission spectroscopy (UPS) taking advantage of a novel multi-channel spin filter. An exceptionally large spin polarization of 93% is obtained at room temperature, providing strong direct evidence for half-metallicity. The energy dependencies of the measured spin polarization as well as of spin integrated UPS essentially agree with bulk band structure calculations. Additional ex-situ spin integrated hard x-ray photoemission spectroscopy experiments (HAXPES) corroborate that indeed bulk states are observed by SRUPS.

15 min. break

MA 11.7 Mon 17:15 BEY 118

Spin dependent lifetimes and non-degenerate spin hot spots in Heusler compounds — •Steffen Kaltenborn and Hans Christian Schneider — Physics Department and Research Center OPTIMAS, University of Kaiserslautern

We present results of an accurate ab-initio calculation of the dielectric function of the half-metallic Heusler compounds Co_2MnSi and Co_2FeSi. The numerical method is based on density functional theory [1,2] in combination with a wave-vector dependent linear tetrahedron method [3]. The dielectric function is used study optical, acoustic and intraband plasmon dispersions in these half metals. As in the case of simple metals, a negative intraband plasmon dispersion [3] is found. Furthermore, we use the dielectric function to analyze the **k** and spin-resolved electronic lifetimes in these materials. Qualitatively, the lifetimes reflect the lineup of electron and hole bands. We determine the spin-flip and spin-conserving contributions to the lifetimes and predict that different excitation conditions may lead to different spin-flip dynamics of excited electrons and may even give rise to an enhancement of the non-equilibrium spin polarization. Finally, we study in detail the behavior of the lifetimes around states that are strongly spin mixed by spin-orbit coupling. We find that, for non-degenerate bands, the spin mixing alone does not determine the energy dependence of the (spin-flip) lifetimes.

[1] DFT-Program The Elk FP-LAPW Code, http://elk.sourceforge.net. [2] C. Ambrosch-Draxl et al., Comp. Phys. Commun. **175**, 1-14, (2006). [3] S. Kaltenborn and H. C. Schneider, Phys. Rev. B **88**, 045124 (2013).

MA 11.8 Mon 17:30 BEY 118

NMR Investigation of Optimal Mn Content in $Co_2Mn_xSi_{0.88}$ Thin Films for High Tunneling Magneto-Resistance — •Steven Rodan[1], Tomoyuki Taira[2], Masafumi Yamamoto[2], Bernd Büchner[1,3], and Sabine Wurmehl[1,3] — [1]Leibniz Institute for Solid State and Materials Research, 01171 Dresden, Germany — [2]Division of Electronics for Informatics, Hokkaido University, Sapporo 060-0814, Japan — [3]Institute für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany

Half-metallic ferromagnets (HMFs), with 100% spin-polarized conduction electrons, are prime candidates for developing spintronics devices. Many Heusler compounds, such as Co_2MnSi, are predicted to be HMFs. A technique for probing local structure such as nuclear magnetic resonance (NMR) is essential for understanding the microscopic origin of manifested physical properties. Local atomic disorder was investigated using both ^{59}Co and ^{55}Mn NMR on epitaxial films of $Co_2Mn_xSi_{0.88}$, with varying Mn content (x = 0.72, 1.12, 1.32). NMR spectra confirmed that the high tunneling magneto-resistance ratio values for magnetic tunnel junctions with electrodes made from highest Mn excess (x=0.32), can be attributed mainly to the reduction of Co antisites (Co on Mn and/or Si sites), which are expected to strongly decrease the half-metallicity.

MA 11.9 Mon 17:45 BEY 118

Evolution of the coercive field of Co_2FeGa Heusler nanocrystals and related oxide nanoparticles inside carbon nanotubes — •Markus Gellesch[1], Usue Palomares Iñiguez de Ciriano[1], Changhai Wang[2], Sabine Wurmehl[1], Silke Hampel[1], and Bernd Büchner[1] — [1]Leibniz Institut für Festkörper- und Werkstoffforschung Dresden — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Magnetic properties of nanoscale systems may differ largely from the magnetism in the respective bulk phase and thus can lead to the emergence of interesting and also novel physical properties. Here we present results of investigations of magnetic properties of Heusler nanoparticles and related oxide materials prepared inside multi-walled carbon nanotubes via a wet-chemical approach. While previous studies[1] already showed, that the coercive field of the Heusler nanocrystals inside carbon nanotubes is enhanced by a factor of at least 30, we now report of an enhancement factor of approximately 100 in Co_2FeGa nanoparticles and of coercive fields as large as 6000 Oe in related oxide materials. Further we present results of the diameter dependence of the coercive field in the later material. The results of our work open the door for the exploration of Heusler and related magnetic materials at the nanoscale and also guide the way to the synthesis of nanomaterials with tailored physical properties.

[1] Gellesch et al., Cryst. Growth Des., 2013, 13 (7), pp 2707–2710

MA 11.10 Mon 18:00 BEY 118

The influence of p- and n-doping on the intrinsic properties of the Heusler compound Fe_2VAl — •Franziska Seifert[1,2], Christian G.F. Blum[1], Frank Steckel[1], Christian Hess[1], Hans-Joachim Grafe[1], Bernd Büchner[1], Sabine Wurmehl[1], Stefan Martin[2], Volker Klemm[2], and David Rafaja[2] — [1]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [2]TU Bergakademie Freiberg, Germany

In this work, we studied the intrinsic properties of the Heusler compound Fe_2VAl and the influence of p (V substituted by Ti)- and n-doping (Al substituted by Si) on the intrinsic materials properties using single crystals. Electron back scattering diffraction reveals the presence of a V-rich secondary ferromagnetic phase in particular in crystals with Si and in the parent compound, which could be further confirmed by TEM investigations. The depletion of V from the Fe_2VAl matrix apparently leads to localized Fe moments and also to magnetic order in the corresponding samples. The evolution of magnetic order and thermoelectric key parameters were further analysed by means of nuclear magnetic resonance, transport and magnetization measurements. Interestingly, the sample with Ti and less V depletion shows a significant enhancement of the figure of merit compared to the other samples.

MA 11.11 Mon 18:15 BEY 118

Effect of high pressures synthesis on $Ba_3YIr_2O_9$ — •Hannes Stummer, Tusharkanti Dey, Sabine Wurmehl, and Bernd Büchner — Leibniz-Institute for Solid State and Materials Research Dresden, Germany

The emergent field of Iridium oxide based materials recently came into focus due to their variety of interesting physical properties, specifically the new and unknown combinations of magnetic properties with interesting ground states [1]. These fascinating phenomena are induced by interaction of large Spin-Orbit-Coupling of the 5d transition metal and the onsite Coulomb energy U. Recent investigations of the Iridate $Ba_3YIr_2O_9$ show that sample grown under normal pressure crystallize in a hexagonal structure and exhibit magnetic ordering below 4 K [2]. The crystal structure is transformed to a cubic double perovskite configuration (stable at ambient pressure), when treated at 8 GPa pressure. In this cubic double perovskite phase the magnetic ordering is suppressed. A possible spin-orbit driven spin liquid ground state is proposed for the high pressure perovskite structure [3]. We will present recent results about the systematic high pressure synthesis of $Ba_3YIr_2O_9$ samples grown under different growth pressure in a Multi-Anvil assembly.The main focus will be on the measurements of structural and magnetic properties depending on the applied pressure during the synthesis process. [1] B. J. Kim et al., Phys. Rev. Lett. 101, 076402 (2008) [2] Y. Doi et al., J. Phys.: Condens. Matter 16, 2849 (2004) [3] T. Dey et al., Phys. Rev. B 88, 134425 (2013)

MA 11.12 Mon 18:30 BEY 118

Pressure-tuning of the magnetic properties of the zero-field cooled exchange-bias Heusler compound Mn_2PtGa — •Catalina Salazar, Ajaya K. Nayak, Claudia Felser, and Michael Nicklas — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

The Heusler compound Mn_2PtGa crystallizes in a tetragonal structure at room temperature. It undergoes a paramagnetic to ferrimagnetic (FI) transition around T_c=230 K followed by a first-order ferrimagnetic to antiferromagnetic (AFM) transition at lower temperature. The most intriguing feature observed in Mn_2PtGa is, however, a large zero-field cooled exchange bias. Here, we present a study of the pressure evolution of the magnetic properties of the Mn_2PtGa Heusler alloy by magnetization measurements under hydrostatic pressures up to 1.2 GPa.