MA 3: Magnetic Half Metals and Oxides

Time: Monday 11:00–13:15 Location: HSZ 401

MA 3.1 Mon 11:00 HSZ 401

Magneto-optical study of Co_2-based Heusler compound thin films — •Simon Trudel, Jaroslav Hamrle, Oksana Gaier, Thomas Sebastian, and Burkard Hillebrands — FB Physik and Forschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany

Co_2-based Heusler compounds are promising materials for spintronic applications due to their predicted half-metallicity, their high Curie temperatures, and their tunable magnetic properties with respect to composition.

In this presentation, we will present our recent results on the magnetic characterization of Co_2-based Heusler compound thin films using magneto-optical probes such as magneto-optical Kerr effect (MOKE) and Brillouin light scattering (BLS) spectroscopy.

In our MOKE investigations, we particularly focus on the amplitude of the longitudinal (LMOKE) and quadratic MOKE (QMOKE) signals. We find that for several Co_2-based Heusler alloys, the QMOKE signal is remarkably strong. This points to an important contribution from second-order (and higher) spin-orbit interaction in this family of materials.

Using BLS spectroscopy, we find that the exchange constant of Co_2-based compounds depends on their composition. In particular, the exchange constant and the spin-wave exchange stiffness increase with the concentration of valence electrons.

Financial support from DFG FG559 "Neue Materialien mit hoher Spinpolarization"is gratefully acknowledged.

MA 3.2 Mon 11:15 HSZ 401

Surface properties of Co based full Heusler alloys — •Jan-Peter Wüstenberg, Sabine Neuschwander, Alexander Fischer, Martin Aeschlimann, and Mirko Cinchetti — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin Schrödingerstr. 46, 67663 Kaiserslautern, Germany

Half metallic Heusler compounds are promising candidates for spintronics applications due to their predicted minority spin gap at the Fermi energy. Unfortunately, the proof of half metallicity at the surface is still missing. In this contribution we present spin resolved low energy photoemission data as well as results from LEED and Auger spectroscopy of several Co based full Heusler alloys. The influence of a thin MgO tunneling barrier and small coverages of the organic semiconductor copper-phthalocyanine (CuPC) on the surface spin polarization is discussed and compared to results of the free Heusler surface.

MA 3.3 Mon 11:30 HSZ 401

Investigation of the metal-insulator transition in a thin manganite film by STM/STS — •Christin Kalkert, Vasily Moshnyaga, Bernd Damaschke, and Konrad Samwer — I. Phys. Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The colossal magnetoresistance (CMR) effect in manganite thin films is accompanied by a metal to insulator transition (MIT) in these samples. In this work a thin film of (La1-0.375Pr0.375)0.7Ca0.3MnO3 was grown by the metal-organic aerosol deposition technique on MgO substrates and investigated by transport measurements and scanning tunnelling microscopy (STM) and spectroscopy (STS) as a function of temperature. With these techniques we were able to compare the local electronic properties of the film with the global transport behavior. We observed an electronic phase separation at low temperatures and in the vicinity of the MIT. The metallic conductivity at low temperatures can be attributed to a double exchange mechanism while the insulating regions can be interpreted by a charge ordered high temperature phase.

This work is supported by DFG via SFB 602, TPA2 and the Leibniz program

MA 3.4 Mon 11:45 HSZ 401

Correlation effects in p-electron magnets: the case of RbO_2 — •Roman Kováčik and Claude Ederer — School of Physics, Trinity College Dublin, Dublin 2, Ireland

The development of spintronics in recent years has triggered a need for new materials such as half metallic (HM) ferromagnets. HM materials with 2p-magnetism were proposed from electronic structure calculations, e.g. Rb_4O_6 [1]. However, recent measurements indicate that Rb_4O_6 is a magnetically frustrated system that exhibits spin-glass-like behavior in a magnetic field [2]. This discrepancy was attributed to inadequate treatment of the molecular states within the local spin density approximation (LSDA). This assumption was supported by calculations for RbO_2, known to be an insulating antiferromagnet, which turns out to be HM in LSDA as well. According to [2], this outcome could not be corrected within LDA+U even for $U = 13.6\,\mathrm{eV}$.

We present results of LDA+U calculations for RbO_2, which show that, when allowing the system to reduce its symmetry, an orbitally polarized insulating state is favored for $U > 2\,\mathrm{eV}$, consistent with experiment. Furthermore, we discuss an alternative treatment of on-site correlations in RbO_2, using an effective tight-binding model corresponding to a molecular orbital basis, which is constructed via maximally localized Wannier functions. In this case, the insulating state is obtained for significantly lower $U > 0.5\,\mathrm{eV}$. In addition, we discuss a possible orbital ordering driven by correlation effects.

[1] J. J. Attema *et al.*, J. Am. Chem. Soc. **127**, 16325 (2005).
[2] J. Winterlik *et al.*, J. Phys. Condens. Matter **19**, 1 (2007).

MA 3.5 Mon 12:00 HSZ 401

Photolitchemically deposited amorphous iron(III) oxide exhibiting room-temperature ferromagnetism — •Simon Trudel[1,2] and Ross H. Hill[1] — [1]4D LABS and Department of Chemistry, Burnaby, BC, Canada — [2]Now at FB Physik and Forschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany

There is great interest in the study of new materials that exhibit useful ferromagnetic properties, while they are expected to be non-magnetic. A surprising example is amorphous iron oxide (a-Fe_2O_3), for which room temperature ferromagnetism (FM) has never been reported.

Thin films of a-Fe_2O_3 were prepared using a photochemical deposition method that allows direct patterning, without the use of photoresists. This method relies on light-induced decomposition of Fe(III) 2-ethylhexanoate, which can be spin-coated as high-quality thin films. Upon exposure to light, the precursor decomposes, yielding a-Fe_2O_3. The a-Fe_2O_3 thin films were found to exhibit FM at room temperature. Prior to this work, no magnetic amorphous iron oxide had previously been reported (*J. Phys. Chem. B* **111** (2007) 4003).

The FM in these films can be tuned by changing the preparation conditions, and complete deactivation of the FM can be achieved by changing the deposition temperature. The oxidation state and coordination of the Fe centers in a-Fe_2O_3 were detemined using X-ray absorption spectroscopy. It will be shown this route to amorphous magnetic oxide materials is general, and that a-Cr_2O_3 and a-$CoFe_2O_4$ also exhibit unprecedented room-temperature FM.

MA 3.6 Mon 12:15 HSZ 401

Phase transition and anomalous low temperature ferromagnetic phase in a $Pr_{0.6}Sr_{0.4}MnO_3$ single crystal — •Sahana Roessler[1], Steffen Wirth[1], Frank Steglich[1], S Harikrishnan[2], C. M. Naveen Kumar[2], Suja Elizabeth[2], H. L. Bhat[2], and Ulrich Karl Roessler[3] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [2]Department of Physics, Indian Institute of Science, Bangalore 560012, India — [3]IFW Dresden, Postfach 270016, D-01171 Dresden, Germany

We report on the specific heat, electrical and magnetic properties of a $Pr_{0.6}Sr_{0.4}MnO_3$ single crystal. This compound is ferromagnetic and metallic below 300 K. The critical properties of the ferromagnetic transition investigated by static magnetic measurements, resistivity and specific heat display a continuous phase transition with the critical exponents belonging to those of the Heisenberg universality class. However, below a structural transition at $T_S \sim 60$ K, the field dependence of magnetization (M-H) loops display anomalous behavior, with the virgin curve lying outside the subsequent M-H cycles. The coercivity of these M-H loops is found to be close to zero. The hysteretic transformation and irreversible magnetization processes below T_S is explained by phase separation between the orthorhombic and monoclinic ferromagnetic phases. Magnetic fields apparently drive modifications in these phase-separated microstructures which suggests a high magnetic anisotropy of the monoclinic phase.

MA 3.7 Mon 12:30 HSZ 401

Magnetism without magnetic impurities in oxides ZrO2 and TiO2 — •Frantisek Maca[1], Josef Kudrnovsky[1], Vaclav Drchal[2], and Georges Bouzerar[2,3] — [1]Institute of Physics ASCR, Praha, Czech Republic — [2]Institut Néel, CNRS, Grenoble, France — [3]Institut Laue Langevin, Grenoble France

We perform a theoretical study of the magnetism induced in transition metal dioxides ZrO2 and TiO2 by substitution of the cation by a vacancy or an impurity from the groups 1A or 2A of the periodic table, where the impurity is either K or Ca.

In the present study both supercell and embedded cluster methods are used. It is demonstrated that the vacancy and the K-impurity leads to a robust induced magnetic moment on the surrounding O-atoms for both the cubic ZrO2 and rutile TiO2 host crystals. The presence of an impurity band close to the top of the valence band is a precursor for the appearance of magnetism in dioxides.

[1] F. Maca, J. Kudrnovsky, V. Drchal, and G. Bouzerar, Appl. Phys. Lett. 92, 212503 (2008).

MA 3.8 Mon 12:45 HSZ 401

Effect of strain and magnetic interaction parameters in Fe_2O_3-$FeTiO_3$ heterostructures — •Hasan Sadat Nabi and Rossitza Pentcheva — Department of Earth and Environmental Sciences, University of Munich, Theresienstr. 41, 80333 Munich, Germany

The interfaces between complex oxides provide a challenging area to explore new functionality for the development of future devices. To explain the origin of interface magnetism in the Fe_2O_3 (canted antiferromanet)- $FeTiO_3$ (room temperature paramagnet) system we have performed density functional theory (DFT) calculation including a Hubbard U parameter. We find that the polar discontinuity at the interface is accommodated through a disproportionation in the Fe contact layer into Fe^{2+}, Fe^{3+}[1] giving the first theoretical evidence for the lamellar magnetism hypothesis [2].

Furthermore, by using the lateral lattice constant of different substrates (e.g. Fe_2O_3, $FeTiO_3$, Al_2O_3) we show how the electronic properties and energetic stability of the system can be tuned by strain. In addition, the magnetic exchange interaction parameters are extracted by mapping the DFT total energies of different spin-configurations on a Heisenberg Hamiltonian.

Funding by the German Science Foundation (DFG PE883/4-1), ESF (EuroMinSci-MICROMAGN) and a grant for computational time at the Leibniz Rechenzentrum are gratefully acknowledged.

[1] R. Pentcheva, H. Sadat Nabi, Phys. Rev. B, **77**, 172405 (2008).
[2] Robinson, P. *et al.* Nature **418**, 517 (2002).

MA 3.9 Mon 13:00 HSZ 401

Ultrafine nc-NiO: a Néel-type Random Ferrimagnet? — •Marek Petrik and Bernd Harbrecht — Chemistry Department and Center of Materials Science, Philipps University, Hans-Meerwein-Strasse, 35032 Marburg, Germany

Is ultrafine nanocrystalline nickel oxide nc-NiO an intrinsic random ferrimagnet as hypothesized by Louis Néel in 1962 [1]? Or is the often reported uncompensated magnetic moment of this archetypal antiferromagnet in the finely divided state due to some other cause? The question has never been conclusively settled in spite of efforts by the groups of Richardson [2], Mørup [3], Seehra [4], and others. Unable to locate the uncompensated spins in nc-NiO directly, we have resorted to indirect means of identifying their origin [5]. Since the magnetism is strongly correlated with the crystallite size and shape, we control these two in a novel solid-state synthesis in the full mesoscopic range (2,5-50 nm). An analysis of the Langevin-type superparamagnetism and the Néel-Arrhenius thermal relaxation, as a function of size, for a large number of samples indicates that nc-NiO not only is a random ferrimagnet as considered by Néel, but also that it could either be subject to a size-dependent magneto-crystalline anisotropy or even consist of multiple antiferromagnetic nanodomains. – [1] L. Néel, in Low Temperature Physics, C. De Witt et al., eds., Gordon and Breach, New York, 1962, p. 412. - [2] J. T. Richardson et al, J. Appl. Phys., 70 (1991) 6977. - [3] C. R. H. Bahl et al., J. Phys.: Condens. Matter, 18 (2006) 4161. - [4] H. Shim et al., Solid State Comm., 145 (2008) 192. - [5] M. Petrik, B. Harbrecht, Z. Anorg. Allg. Chem., 634 (2008) 2069.