MA 17 Magnetic Materials II

Time: Tuesday 10:15–13:00 Room: HSZ 401

MA 17.1 Tue 10:15 HSZ 401

Magnetism without d-electrons — •Martin Sieberer, Josef Redinger, Sergii Khmelevskyi, and Peter Mohn — Center for Computational Materials Science, Vienna University of Technology, Getreidemarkt 9/134, A-1060 Vienna, Austria

On the basis of ab-initio calculations employing density functional theory (DFT) we investigate half metallic ferromagnetism in zinc-blende and wurtzite compounds composed of group I/II metals as cations and group V elements as anions. We find that the formation of ferromagentic order requires large cell volumes, high ionicity and a slight hybridization of anion p and cation d states around the Fermi energy. Our calculations show that a ferromagnetic alignment of the spins is energetically always more stable than simple AF arrangements, which makes these materials possible candidates for spin injection in spintronic devices. To clarify the conditions for the flat p-band carrying the magnetism, we present results of a tight binding analysis.

MA 17.2 Tue 10:30 HSZ 401

Complex magnetic order and transition to half-metallicity in Mn-doped Fe_3Si — •Phivos Mavropoulos, Marjana Ležaić, and Stefan Blügel — IFF, Forschungszentrum Jülich, D-52425 Jülich, Germany

Fe_3Si is a ferromagnetic material with possible applications in magnetic tunnel junctions [1]. When doped with Mn, the material shows a complex magnetic behavior, as suggested by older experiments [2]. Motivated by the above, we employed the Korringa-Kohn-Rostoker Green function method within density-functional theory in order to study the alloy $Fe_{3-x}Mn_xSi$, with $0 \leq x \leq 1$. The Mn atoms are positioned at the octahedral site of the $L2_1$ crystal structure. Chemical disorder is described within the coherent potential approximation (CPA); magnetic disorder is considered within the disordered local moment (DLM) state, again using the CPA. We find that, for $x \leq 0.3$, the Mn atoms align antiferomagnetically ($Mn^{\downarrow}$) to the Fe atoms, while for $x \geq 0.75$ the alignment is ferromagnetic ($Mn^{\uparrow}$). For intermediate Mn concentrations, the energy minimum is at a DLM state of the form $Fe_{3-x}(Mn^{\downarrow}_{x-y}Mn^{\uparrow}_{y})Si$, in which only a fraction y of the Mn atoms is ferromagnetically coupled to Fe. In the concentrated limit ($x = 1$), the (ordered) alloy is half-metallic. For lower concentrations the spin polarization at the Fermi level is also considerable: for $x = 0.65$, $P = 0.93$, and for $x = 0.55$, $P = 0.85$.

We discuss the origin of the transition to ferromagnetic behavior, the exchange interactions and the spin polarization.

[1] A. Ionescu et al., Phys. Rev. B **71**, 094401 (2005)
[2] S. Yoon and J. G. Booth, J. Phys. F: Met. Phys. **7**, 1079 (1977)

MA 17.3 Tue 10:45 HSZ 401

XMCD study of the 5*d* magnetism at the B′ site in double perovskites $A_2CrB'O_6$ — •P. Majewski[1], S. Geprägs[1], O. Sanganas[1], M. Opel[1], R. Gross[1], G. Vaitheeswaran[2], V. Kanchana[2], A. Delin[2], F. Wilhelm[3], A. Rogalev[3], and L. Alff[4] — [1]Walther-Meissner-Institut, Bavarian Academy of Sciences, Walther-Meissner-Str. 8, 85748 Garching, Germany — [2]Department of Materials Science and Engineering, Royal Institute of Technology (KTH), 10044 Stockholm, Sweden — [3]European Synchrotron Radiation Facility (ESRF), 6 Rue Jules Horowitz, BP 220, 38043 Grenoble, Cedex 9, France — [4]Darmstadt University of Technology, Petersenstr. 23, 64287 Darmstadt, Germany

We have investigated the magnetic moment of the ′non-magnetic′ B′ ion W (resp. Re) in the ferrimagnetic double perovskites Sr_2CrWO_6, Ca_2CrWO_6 and Sr_2CrReO_6 by X-ray magnetic circular dichroism (XMCD) at the L2/3 edges. In all compounds, a negative spin and a positive orbital moment for the B′ ion was detected. Our results are in good agreement with recent band-structure calculations and confirm that the magnetism in these materials is determined by an electronic configuration with localized, highspin 3*d* electrons on the magnetic ion (Cr) and delocalized 5*d* electrons on the ′non-magnetic′ site, which are polarized antiparallel. We find that these double perovskites follow the scaling law of the spin magnetic moment at the site of the ′non-magnetic′ B′ ion with Curie temperature.

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MA 17.4 Tue 11:00 HSZ 401

Rare-earth ferroborates $RFe_3(BO_3)_4$: A novel route to multiferroism — •R. Klingeler[1], C. Hess[1], N. Tristan[1], Y. Skourski[1], B. Büchner[1], E. Popova[2], A. Vasiliev[2], L.N. Bezmaternykh[3], N.A. Stolbovaya[3], and V.L. Temerov[3] — [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden, Postfach 270116, — [2]Faculty of Physics, M.V. Lomonosov, Moscow State University, — [3]L.V. Kirensky Institute of Physics, Siberian

$GdFe_3(BO_3)_4$ is known to be a new multiferroic compound since it exhibits both ferroelectric and antiferromagnetic properties. Little is known about other members of the $RFe_3(BO_3)_4$ family (R=Eu, Tb, Dy, Ho, ...). We report on thermodynamic properties of Tb- and Y based compounds, i.e. specific heat and magnetization measurements in high magnetic fields and in a wide temperature range.

MA 17.5 Tue 11:15 HSZ 401

Direct imaging of stripe-like features in $La_{0.75}Ca_{0.25}MnO_{3-y}$ by scanning tunneling microscopy — •Lakshmana Sudheendra[1], Vasily Moshnyaga[1], Sigrun Koester[1], Kai Gehrke[1], Bernd Damaschke[1], O Shapoval[2], A Belenchuk[2], and Konrad Samwer[1] — [1]I. Physikalisches Institut, University of Goettingen, Friedrich-Hund-Platz 1, D-37077, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, Academiei Str. 5, MD-2028, Chisinau, Moldova

We have performed high resolution scanning tunneling microscopy (STM) and spectroscopy on pseudo-cubic and orthorhombic $La_{0.75}Ca_{0.25}MnO_{3-y}$ films. In the ferromagnetic regime, we observe stripe-like features for the pseudo-cubic film. The typical stripe dimensions are 3-5 unit cells. This charge-stripe dimension observed under STM is consistent with the length scale of 'correlated polarons' observed in manganites from various diffraction techniques [1]. The room temperature images show unusual charge modulation at the atomic scale. The formation of stripes and the unusual charge modulations are discussed based on the charge, orbital and the vacancy ordering [2]. The orthorhombic film, on the other hand, shows stripe-like features at room temperature, which is consistent with the stabilization of the polarons due to the greater structural distortion.

Acknowledgement: We acknowledge the support of DFG-SFB 602 TP A2, the Leibniz programm and the A.v Humboldt foundation (L.S)

1. R. Kajimoto et al., Phys. Rev. B 66, 180402(R) (2002) 2. Takashi Hotta et al., Phys. Rev. Lett. 86, 4922 (2001)

MA 17.6 Tue 11:30 HSZ 401

Electronic structure of highly ordered Sr_2FeMoO_6: XPS and XES studies — •K. Kuepper[1,2], M. Kadiroglu[2], A. V. Postnikov[2,3], K. C Prince[4,5], M. Matteucci[6], V. R. Galakhov[3], H. Hesse[2], G. Borstel[2], and M. Neumann[2] — [1]Forschungszentrum Rossendorf e. V., D-01328 Dresden, Germany — [2]University of Osnabrück, Department of Physics, D-49069 Osnabrück, Germany — [3]Institute of Metal Physics, 620219 Yekaterinburg GSP-170, Russia — [4]Laboratorio TASC-INFM, I-34012 Basovizza (Trieste), Italy — [5]Sincrotrone Trieste, I-34012 Basovizza (Trieste), Italy — [6]ICGEB, I-34012 Trieste, Italy

We have investigated the electronic structure of Sr_2FeMoO_6. In order to probe the partial densities of states we applied soft x-ray emission spectroscopy (XES) to the Fe *L*, the Mo *M* and the O *K* edges. We discuss the results in the light of complementary measurements of the valence band by means of x-ray photoelectron spectroscopy (XPS) and first-principles generalized gradient approximation (GGA) and LDA + U band structure calculations [1].

[1] K. Kuepper *et al.*, J. Phys.: Condens. Matter **17**, 4309 (2005).

MA 17.7 Tue 11:45 HSZ 401

Microscopic magnetism of the multiferroic spinel CdCr2S4 — •E. Goering[1], S. Gold[1], J. Deisenhofer[2], J. Hemberger[2], V. Tsurkan[2], and A. Loidl[2] — [1]MPI für Metallforschung, 70569 Stuttgart — [2]Institiut für Korrelationen und Magnetismus, Uni-Augsburg, 86135 Augsburg

The coexistence of ferromagnetism and ferroelectricity, has recently attracted much interest in perovskite rear earth manganites [1]. This is connected to a possible new generation of promising electronic devices,

where electronic polarization and magnetism are coupled to each other. For CdCr2S4 a colossal magnetocapacitive coupling has been observed close to the ferromagnetic ordering temperature of about [2]. We will show here X-ray magnetic circular dichroism results at the Cr L2,3 edges performed at 33K and 1T external magnetic field, in order to investigate the microscopic magnetic properties of CdCr2S4. The magnetic spectra exhibit unusual and very complex structures (see figure). By the use of sum rules and a self consistent j3/2 j1/2 mixing correction a slightly reduced, compared to the bulk value of 3*B [2], spin moment of 2.2*B has been found. The orbital moment exhibits a nearly vanishing value of 0.037*B, consistent to the theoretically predicted high spin configuration with fully occupied majority t2g orbitals.

[1] T. Kimura, et al.; Nature 426 (2003) 55. T. Goto, et al.; Phys. Rev. Lett 92 (2004) 257201 [2] J. Hemberger, et al.; Nature 434 (2005) 364.

MA 17.8 Tue 12:00 HSZ 401

Characterization of boron-free Fe-based metallic glasses using small-angle neutron scattering — •Giovanni Mastrogiacomo[1], Joachim Kohlbrecher[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, Swiss Federal Institute of Technology (ETH) Zürich, Wolfgang-Pauli-Strasse 10, CH-8093 Zürich, Switzerland — [2]Paul Scherrer Institute, CH-5232 Villigen-PSI, Switzerland

According to structural models, the development of Fe-based metallic glasses is strongly correlated to the amount of metalloids. However, a higher amount of metalloids causes deterioration not only in magnetic properties but also in plasticity. Starting from a Fe-Cr-Co system, which exhibits a decomposing tendency in the solid state, several boron-free Fe-based metallic glasses of composition (Fe0.582Co0.418)100-x-yCrxZry (10<x<28 and 8<y<11) were developed. The development of these alloys was based on destabilization of the solid state via the application of the Hume-Rothery rule, where low solubility is achieved for alloying elements with atomic size ratios differing by more than 15%. Alloying of zirconium in the Fe-Cr-Co system, which satisfies the Hume-Rothery rule, causes a decrease in the liquidus temperature. The resulting magnetization measurements of a boron-free Fe-based metallic glass of composition (Fe0.582Co0.418)80Cr10Zr10 reveal a saturation magnetization of up to 1.1 T and an inverted hysteresis. According to small-angle neutron scattering measurements, the inverted hysteresis can be attributed to the presence of two phases, resulting from the decomposing tendency of the Fe-Cr-Co system.

MA 17.9 Tue 12:15 HSZ 401

Orbital magnetic moment anisotropy in (GaMn)As — •F. Kronast[1], R. Ovsyannikov[1], A. Vollmer[1], H.A. Dürr[1], W. Eberhardt[1], G.M. Schott[2], C. Ruester[2], C. Gould[2], G. Schmidt[2], K. Brunner[2], L.W. Molenkamp[2], and J. Cesar[3] — [1]BESSY GmbH, Albert Einstein Strasse 15, 12489 Berlin, Germany — [2]Physikalisches Institut III, Universität Würzburg, Germany — [3]ESRF, BP 220, 38043 Grenoble Cedex, France

Using x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD) we studied the ferromagentic ordering in (GaMn)As, the most prominent member of the III-V series of ferromagnetic dilute magnetic semiconductors (DMS). Mn replacing the trivalent Ga atoms provides a local spin magnetic moment and as an acceptor it creates itinerant holes [1]. The exchange coupling of holes to the Mn 3d shell by pd-hybridization mediates the long range ferromagnetic order. The pd-hybridization is usually assumed to be spherically isotropic [2].

Only recently Mahadevan et al. predicted a strongly anisotropic pd-hybridization due to p-d hopping interactions that depend on the specific lattice orientation (Phys. Rev. Lett., 93, 177201, 2004). In angle dependent XMCD measurements we find a variation of the Mn 3d orbital moment with the in-plane azimuthal lattice direction that is correlated with distinct spectroscopic features. Both can be interpreted by a spin-orientation dependent spatial anisotropy of the Mn acceptor state influencing the ferromagnetic ordering. This is the first experimental indication for an anisotropic pd-hybridization in (GaMn)As and, therefore, magnetic exchange coupling.

MA 17.10 Tue 12:30 HSZ 401

Crystal growth and physical properties of cuprates grown under high pressure — •Nadja Wizent[1], Günther Behr[1], Lutz Schramm[1], Mircea Apostu[1], Anja Waske[1], Thomas Doerte[2], Michael Ruck[2], Bernd Büchner[1], and Wolfgang Löser[1] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany — [2]Technische Universität Dresden Institut für Anorganische Chemie Dresden, Germany

The copper oxide-based compounds are known for interesting properties like superconductivity, spin and charge ordering. Single crystals of cuprates with Co and Ca were grown with the travelling floating zone method under high oxygen pressure. Phase diagram studies were carried out on the basis of CALPHAD calculations. Magnetic and heat capacity measurements were accomplished on as grown and annealed crystals. Different growth strategies and heat treatments for the metastable phase $CoCu_2O_3$ were elaborated, which show the striking effect of growth rate on the constitution. A $CaCu_2O_3$ type phase was grown under 50 bar oxygen pressure with the composition of $(Ca_{0,75}Cu_{0,25})Cu_2O_3$. Magnetic measurements revealed antiferromagnetic ordering below T_N= 31 K . From structure investigations it is concluded that 11% of all Cu-atoms are on Ca-sites. Whereas, only 1/3 of them display magnetic moments.

MA 17.11 Tue 12:45 HSZ 401

Influence of texture on corrosion behaviour of highly anisotropic sintered magnets — •Mihaela Rada[1], Annett Gebert[1], Irina Mazilu[1], Kirill Khlopkov[1], Oliver Gutfleisch[1], Ludwig Schultz[1], and Werner Rodewald[2] — [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany — [2]Vacuumschmelze GmbH & Co KG, P.O. Box, D-63412 Hanau, Germany

The anisotropic corrosion behaviour of highly textured sintered Nd-Fe-B magnets in weakly acidic solutions has been evaluated by investigations of magnet surfaces, which are parallel or perpendicular to the crystallographic c-axis of the aligned ferromagnetic grains. The total corrosion process progresses more pronouncedly at the perpendicular magnets surfaces (the pole faces). Under free corrosion and anodic polarization conditions the parallel magnet surfaces exhibit a stronger active dissolution tendency due to an enhanced reactivity of grain surfaces parallel to the (100) plane of the Nd2Fe14B crystals. Single misoriented grains dissolve preferentially at both magnet sides. Under cathodic conditions the hydrogenation process progresses more rapidly at the perpendicular sides, suggesting a local preferential penetration of atomic hydrogen into the material.