# MA 10: Magnetic Materials

Time: Monday 15:15–18:30 Location: H 1028

MA 10.1 Mon 15:15 H 1028

**Spin Density Wave state in Chromium: density functional calculations** — •Mathias Bayer, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

The ground state of Chromium is an incommensurable spin density wave with a period of about 42 atomic layers. Recent electronic structure calculations for Cr, including up to 40 layers, found an anti-ferromagnetic groundstate. We have used the full-potential local-orbital code FPLO, which has allowed us to consider up to 42 layers at a high accuracy of the total energy in LSDA. We have additionally applied a lattice distortion to simulate the effects of the concomitant charge density wave. The results are compared with experimental data and other calculations in the literature.

MA 10.2 Mon 15:30 H 1028

**Temperature induced changes of the Ni electronic structure** — •Ruslan Ovsyannikov, Mihaela Gorgoi, Florian Kronast, Hermann A. Dürr, and Wolfgang Eberhardt — BESSY GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Temperature dependent changes for surface and bulk states in valence band photoemission are well known [1] and often assigned to an expanding lattice. A similar explanation was proposed for core levels of transition metals such as W [2]. Here we show that the crystalline field is not the only origin of a temperature induced core level shifts. We show using bulk sensitive high kinetic energy photoemission that in the case of Ni a more pronounced temperature effect is visible in core level satellites compared to the main peak. A similar behavior is also observed with XAS. We discuss a model where this behavior can be explained by a reduced hybridization between 3*d* and 4*sp* orbitals on neighbor Ni atoms with increasing temperature.

[1] R. Paniago et al., J. Phys.: Condens. Matter 7, 2095 (1995)
[2] H.-S. Tao et al., Phys. Rev. B 56, 6982 - 6986 (1997)

MA 10.3 Mon 15:45 H 1028

**Magnetic and thermodynamic properties of the frustrated ferromagnetic square lattice $BaCdVO(PO_4)_2$** — •Ramesh Nath[1], A. A. Tsirlin[1,2], H. Rosner[1], and C. Geibel[1] — [1]MPI CPfS, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Department of Chemistry, Moscow State University, 119992, Moscow, Russia

The spin 1/2 Heisenberg model on a square lattice with antiferromagnetic (AF) nearest $J_1$ and next nearest neighbour $J_2$ interactions has been a focus of extensive theoretical research for the last decades. Experimentally, only a limited number of compounds of this model have been realized so far. Very recently new materials, $(Pb_2, SrZn)VO(PO_4)_2$ were found to be square lattice systems with mixed ferromagnetic (F) and AF exchange interactions which stimulated the theoretical research to extend the phase diagram including F $J_1$ and $J_2$. In this context, we would like to present a new compound $BaCdVO(PO_4)_2$, which is isostructural to $SrZnVO(PO_4)_2$ and more exciting from the magnetic point of view. Magnetization and specific heat measurements on powder sample evidence that $BaCdVO(PO_4)_2$ is a $S = 1/2$ frustrated square lattice with F $J_1$ and AF $J_2$. The absolute values were estimated to be $J_1 \simeq -3.6$ K and $J_2 \simeq 3.2$ K which are consistent with a strongly reduced (or vanishing) Curie temperature $\theta_{CW}$. $BaCdVO(PO_4)_2$ undergoes a magnetic ordering at about 1 K, likely towards a columnar antiferromagnetic state as expected from the ratio $J_2/J_1 \simeq -0.85$ and the saturation field $B_{sat} \simeq 4.5$ T. This ratio, places the system more close to the quantum critical regime in the phase diagram than previously reported compounds.

MA 10.4 Mon 16:00 H 1028

**Simultaneous magnetoresistance measurements and Kerr microscopy of iron whiskers** — •Michael Kirsch, Ivo Knittel, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O.Box 151150, D-66041

Measurements of magnetoresistance and (giant) magnetoimpedance of single crystals have been carried out at room temperature as a function of applied longitudinal magnetic field, current amplitude and current frequency. Simultaneously, the magnetic surface domain structure of the probes was imaged by Kerr microscopy (MOKE). Iron whiskers of 70 to 105 micrometer in diameter with <100> and <111> growing directions have been used for the experiments. Crystallography, zero-field domain structure and MOKE imaging properties will be discussed in detail. The correlation between circumferential magnetic permeability, magnetoimpedance and magnetoresistive effects is discussed on the basis of MOKE and resistivity data. The results permit to model changes of the domain structure during the magnetoimpedance measurement. Magnetoimpedance in iron whiskers can be understood in close analogy to the "giant magnetoimpedance" known from amorphous wires with a "bamboo" domain structure.

MA 10.5 Mon 16:15 H 1028

**Magnetism in $Pb_3Mn_7O_{15}$** — •J. C. E. Rasch[1,2], D. Cheptiakov[2], M. Boehm[1], J. Schefer[2], N. V. Volkov[3], K. A. Sablina[3], and G. A. Petrakovskii[3] — [1]Institut Laue-Langevin, 6 rue Jules Horowitz, BP 156, 38042 Grenoble, Cedex 9, France — [2]Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [3]L.V. Kirensky Institute of Physics SB RAS, Krasnoyarsk 660036, Russia

The wide variety of physical properties in perovskite manganites stimulates the study of other Mn oxide families without perovskite structure, but a mixed valence state of the Mn ions ($Mn^{3+}/Mn^{4+}$).The material under investigation is the quasi 2D compound $Pb_3Mn_7O_{15}$. Both existing models describing the crystal structure [1,2] were disproved and a new model based on the orthorhombic space group *Pnma* could be identified. Magnetisation measurements give evidence of strong antiferromagnetic correlations. A huge step at $T = 70$ K indicates a 3D long range ordered state and a second smaller step at $T = 20$ K is interpreted as reorientation of some moments due to a variation of the magnetic anisotropy with temperature. Neutron single crystal and powder diffraction measurements revealed two magnetic phases in $PbO$-$MnO_2$-$Mn_2O_3$ indicating the presence of different oxidation states. The disappearance of magnetic peaks at $T = 20$ K and $T = 70$ K coincides with the magnetisation measurement. [1] R. E. Marsh, and F. H. Herbstein, Acta Cryst. B **39**, 280 (1983). [2] Y. Le Page, and L. D. Calvert, Acta Cryst. C **40**, 1787 (1984).

MA 10.6 Mon 16:30 H 1028

**Incommensurate Spin Ordering and Fluctuations in Underdoped $La_{2-x}Ba_xCuO_4$** — •Sarah Dunsiger[1], Yang Zhao[2], Bruce Gaulin[2], Hanna Dabkowska[2], Zahra Yamani[3], William Buyers[3], Yiming Qiu[4], John Copley[4], Yvan Sidis[5], and Philippe Bourges[5] — [1]Physics Department E21, Technical University of Munich, D-85748 Garching, Germany — [2]Department of Physics and Astronomy, McMaster University, Hamilton, ON, Canada — [3]Canadian Neutron Beam Centre, NRC, Chalk River Laboratories, Chalk River, ON, Canada — [4]National Institute of Standards and Technology, Gaithersburg, Maryland, USA. — [5]Laboratoire Léon Brillouin, CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France.

The diverse magnetic properties of the $La_{2-x}(Sr,Ba)_xCuO_4$ transition metal oxides may be tuned in a controllable way by doping with mobile holes. In one interpretation, the holes are believed to organise into correlated static or dynamic stripes. We report the first observation of static *incommensurate* spin ordering in underdoped $La_{2-x}Ba_xCuO_4$ (x=0.025, 0.05, 0.08) using neutron diffraction. Elastic collinear incommensurate peaks are observed below the superconducting transition ($T_C \sim 27$ K) in $La_{2-x}Ba_xCuO_4$ (x=0.08). In marked contrast, diagonal satellite peaks have been observed at low temperature in positions rotated by 45° within the (HK0) plane for $La_{2-x}Ba_xCuO_4$ (x∼0.025, 0.05). Our neutron scattering results are compared with analogous studies on $La_{2-x}Sr_xCuO_4$ which indicate that such a rotation of the spin structure may be a generic feature of the underdoped La-214 cuprates.

MA 10.7 Mon 16:45 H 1028

**Electronic, magnetic, and transport properties of quaternary (Cu,Ni)MnSb Heusler alloys** — •Josef Kudrnovsky[1], Vaclav Drchal[1], Peter Weinberger[2], and Patrick Bruno[3] — [1]Institute of Physics AS CR, Prague — [2]Computational Materials Science Center, Vienna — [3]Max-Planck Institut, Halle

Heusler alloy NiMnSb is ferromagnetic halfmetal while its counterpart CuMnSb is the antiferromagnet. The concentration dependence of the the total magnetic moment (resistivity) exhibits a dramatic decrease

(increase) with increasing Cu-concentration starting from about 70% of Cu. On the other hand, the Curie temperature decreases monotonically with the Cu-content. We present the first-principles study of the concentration dependence of magnetic moments, Curie temperatures, and residual resistivities. Results are in a fair agreement with available experimental data. The electronic origin of the observed concentration trends will be also discussed.

MA 10.8 Mon 17:00 H 1028

**Magnetocaloric effect in nickel rich Ni-Mn-Ga Heusler alloys** — Kalyan Mandal[1,2], Julia Lyubina[2], Debabrata Pal[1], Nils Scheerbaum[2], and •Oliver Gutfleisch[2] — [1]Magnetism Laboratory, S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700 098, India — [2]Leibniz Institute für Festkörper- und Werkstoffforschung Dresden (IFW Dresden), Institut für Metallische Werkstoffe, Postfach 270116, 01171 Dresden, Germany

Heusler alloys with nickel-rich compositions Ni(2+x)Mn(1-x)Ga (x=0.16, 0.18, 0.20, 0.22, 0.24, 0.26) have been prepared by arc-melting and subsequent annealing. A large magnetic entropy change, |DS| ˜96 J/Kg.K has been observed around 291 K for the composition Ni(2.22)Mn(0.78)Ga where the martensite-austenite structural transition almost coincides with ferromagnetic-paramagnetic magnetic transition. The effect of hydrostatic pressure up to 8kbar on martensitic transition, magnetic transition and magnetocaloric effect has been studied. The martensitic transition temperature as well as the Curie temperature Tc was found to increase whereas |DS| decreases slightly due to the application of hydrostatic pressure. The large hysteresis observed in M vs H curve at ambient pressure was reduced significantly at 8kbar.

MA 10.9 Mon 17:15 H 1028

**Mößbauer spectroscopy of $Co_2Mn_{1-x}Fe_xAl$.** — •Verena Jung, Gerhard H. Fecher, Benjamin Balke, Vadim Ksenofontov, and Claudia Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz

Heusler compounds have been recognized as suitable materials for magneto-electronics. The $Co_2$ based compounds are of special interest for applications as they exhibit a wide range of magnetic properties and Curie temperatures up to 1100 K. In this work solid solutions of $Co_2Mn_{1-x}Fe_xAl$ with $x = 0, 0.1, \ldots, 1$ were prepared by arc melting and annealed for 7 days at 800°C. The structure was characterized by XRD and a single $B2$ phase was found over the entire range of compositions. The magnetic properties were measured with a SQUID magnetometer revealing that the moments are higher than expected for half-metallic ferromagnetism. The local environment and hyperfine magnetic fields of the iron atoms were studied by $^{57}$Fe Mößbauer spectroscopy in transmission geometry at room temperature for $Co_2Mn_{1-x}Fe_xAl$ samples with $x = 0.2 \ldots 1$. The obtained spectra are explained by hyperfine magnetic field distributions implying 7 contributions with different values and line widths in agreement with the local structure in the cubic lattice. A shift of the relative intensities of the seven hyperfine magnetic fields is explained by the appearance of an additional ordered portion with $L2_1$ structure for samples with Fe concentrations of $x > 0.7$ not being detected by XRD.

The authors gratefully acknowledge financial support by the DfG (Research Unit 559).

MA 10.10 Mon 17:30 H 1028

**High energy high resolution photoemission from Heusler compounds in half tunnelling-junctions.** — •Andrei Gloskovskii[1], Benjamin Balke[1], Siham Ouardi[1], Gerhard H. Fecher[1], Claudia Felser[1], and Masafumi Yamamoto[2] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Graduate School of Informatic Science and Technology, Hokkaido University, Sapporo, Japan.

This work reports on high resolution photoelectron spectroscopy from the valence band of buried $Co_2MnSi$ thin films excited by photons of about 5.9 keV energy. The measurements were performed on $Co_2MnSi$ thin films covered by $MgO(z)/AlO_x(1nm)$ with different thickness $z$ from 2 nm to 20 nm of the MgO interlayer. The film structure corresponds to half a tunnelling magnetoresistive (TMR) junction. It is shown that the high energy spectra reveal the bulk electronic structure of the Heusler compound close to the Fermi energy even through the MgO layer. The high resolution measurements of the valence band close to the Fermi energy indicate a very large electron mean free path of the electrons through the MgO layer. The spectra of the buried thin films agree well with previous measurements from bulk samples.

The authors gratefully acknowledge financial support by the BMBF and DfG (Research Unit 559).

MA 10.11 Mon 17:45 H 1028

**Effect of hydrostatic pressure on the magnetic and magnetocaloric properties of La(Fe,Si)$_{13}$-type alloys** — •Julia Lyubina, Konstantin Nenkov, Kalyan Mandal, Oliver Gutfleisch, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, Helmholtzstr. 20, 01069 Dresden, Germany

The magnetic refrigeration based on the magnetocaloric effect (MCE) is becoming a promising technology to replace the conventional gas-compression/expansion technique. The MCE is the emission or absorption of heat in response to a changing magnetic field and is present in all magnetic materials. A very promising magnetic refrigerator is the $La(Fe,Si)_{13}$ compound, as it shows a giant MCE near room temperature due to a first-order magnetic phase transition. Among important advantages of $LaFe_{13-x}Si_x$ alloys are the reduced hysteresis in melt-spun ribbons[1], the abundance of main constituents and the possibility of adjusting the Curie point $T_c$ by varying x and/or by hydrogenation [2]. In this work, $LaFe_{11.8}Si_{1.2}$ and $LaFe_{11.6}Si_{1.4}$ alloys prepared by melt-spinning and subsequent annealing at 1000 °C/1 h have been studied. The effect of hydrostatic pressure up to 10 kbar on the Curie temperature and itinerant electron metamagnetic transition has been investigated. On applying pressure, a shift of $T_c$ to lower temperatures at a rate of 13 K/kbar is observed. Moreover, it leads to a gradual change from the first- to second-order-type transition. The influence of pressure on the MCE is discussed. [1] O. Gutfleisch et al., J. Appl. Phys. 97 (2005) 10M305. [2] K. Mandal et al., J. Magn. Magn. Mater. 290-291 (2005) 673.

MA 10.12 Mon 18:00 H 1028

**Variation of the Si content and its influence on the structure of rare-earth silicides** — •Tilmann Leisegang[1], Torsten Weissbach[1], Julia Dshemuchadse[1], Christian Graf[2], Thomas Doert[2], Enrico Faulhaber[3], Matthias Frontzek[3], Oliver Stockert[4], Dimitri Souptel[5], Günter Behr[5], Hirale S. Jeevan[4], Christoph Geibel[4], and Dirk C. Meyer[1] — [1]Institut für Strukturphysik — [2]Institut für Anorganische Chemie — [3]Institut für Festkörperphysik — [4]Max-Planck-Institut f. Chemische Physik fester Stoffe — [5]Leibniz-Institut für Werkstoffforschung; Dresden, Germany

Rare-earth silicides (RES) exhibit a large variety of interesting low temperature physical properties depending on the Si content. $CeSi_2$, as an example, exhibits ferromagnetic ordering at low and Kondo behavior at higher Si content. As another example, in $CeCu_2Si_2$, a heavy Fermion compound, the variation of the Si content can result in dominant antiferromagnetic behavior (Si excess) or superconductivity (Si deficiency). To investigate the influence of the Si content on the crystal structure of several RES and to correlate these results with the physical properties, single crystals with certain compositions were synthesised. The investigations were performed by means of single crystal X-ray diffraction and X-ray absorption spectroscopy at ambient conditions. Modulated structures due to vacancy ($CeSi_{1.82}$) and atom ($Ho_2PdSi_3$) ordering were observed as well as specific additional maxima within electron density maps ($CeCu_2Si_2$) indicating stacking fault defects.
We thank the DFG within the SFB 463 for financial support.

MA 10.13 Mon 18:15 H 1028

**Magnetism of the high spin molecules $[Mn_4L_6](BF_4)_2{\cdot}2CH_3CN{\cdot}H_2O$ and $[Cr^{III}Mn^{II}_3(PyA)_6Cl_3]$** — •Manuel Prinz[1], Michael Raekers[1], Karsten Kuepper[2], Phalguni Chaudhuri[3], Simon J. George[4], and Manfred Neumann[1] — [1]Universität Osnabrück, Fachbereich Physik, Barbarastr. 7, D-49069 Osnabrück — [2]FZ Dresden-Rossendorf, Dresden, Germany — [3]MPI, Mülheim an der Ruhr, Germany — [4]LBNL, Berkeley, CA, USA

We have studied the electronic and magnetic structure of high spin molecules by spectroscopic investigations in combination with theoretical calculations. We present results on $[Mn^{II}_4L_6](BF_4)_2{\cdot}2CH_3CN{\cdot}H_2O$ (**$Mn_4$**)and the hetero nuclear, spin frustrated molecule $[Cr^{III}Mn^{II}_3(PyA)_6Cl_3]$ (**$CrMn_3$**), which have been studied using X-ray photoelectron spectroscopy (XPS), X-ray absorption and emission spectroscopy (XAS, XES), and X-ray magnetic circular dichroism (XMCD). Magnetic measurements of **$Mn_4$** show a magnetization saturation of about 20 $\mu_B$/f.u. at a magnetic field of $B = 7$ T and a temperature of $T = 2$ K. From XMCD measurements of **$Mn_4$** at $T = 5$ K and $B = 5$ T we obtained a high magnetic moment of 18.5 $\mu_B$/f.u, whereas a quenching of the Mn orbital moments was observed ($m_{orb} = 0.4$ $\mu_B$/f.u.). The element selective $Mn^{II}$ and

$Cr^{III}$ dichroic signals of the $\mathbf{CrMn_3}$ complex at $B = 5$ T and $T = 5$ K where recorded. For the three $Mn^{II}$ ions a magnetic moment of $\approx 15$ $\mu_B$ was determined. For both complexes we will present a comparison to XAS/XMCD charge transfer multiplet calculations.