

## MA 5 Spin-Structures and Magnetic Phase Transitions I

Time: Monday 10:15–13:00

Room: HSZ 403

MA 5.1 Mon 10:15 HSZ 403

**Field induced incommensurate to commensurate magnetic transition in multiferroic TbMnO<sub>3</sub>** — ●NADIR ALIOUANE, DIMITRI ARGYRIOU, and SVEN LANDSGESELL — Hahn-Meitner-Institut, Glienicke Str. 100, Berlin D-14109, Germany

TbMnO<sub>3</sub> is an improper ferroelectric that exhibits a flop in its electric polarization ( $P$ ) with applied magnetic field ( $H$ ) from  $P||c$  to  $P||a$ . It is argued that ferroelectricity here arises from a spiral spin phase that breaks inversion symmetry. We have used in-field neutron single crystal diffraction to monitor changes in the complex magnetic structure of this material as a function of magnetic field up to 14T and temperature. We show that the flop in the electric polarization that occurs at  $\sim 9$ T and  $\sim 5$ T for  $H$  along the  $a$ - and  $b$ -axis respectively coincides with a 1st order transition to a commensurate magnetic phase with propagation vector  $(0, \frac{1}{4}, 0)$ . On the basis of this commensurate magnetic phase we propose a model of structural distortions that correctly predicts the polarization direction of the high field phase.

MA 5.2 Mon 10:30 HSZ 403

**Magnetic field induced linear magneto-elastic coupling in multiferroic TbMnO<sub>3</sub>** — ●J. STREMPFER<sup>1</sup>, N. ALIOUANE<sup>2</sup>, B. BOHNBUCK<sup>1</sup>, D. ARGYRIOU<sup>2</sup>, I. ZEGKINOGLU<sup>1</sup>, and M. VON ZIMMERMANN<sup>3</sup> — <sup>1</sup>MPI/FKF, Heisenbergstr. 1, 70569 Stuttgart — <sup>2</sup>HMI, Glienicke Str. 100, 14109 Berlin — <sup>3</sup>HASYLAB/DESY, Notkestr. 85, 22605 Hamburg

The multiferroic compound TbMnO<sub>3</sub> was investigated in high magnetic fields up to 10T using high-energy x-ray diffraction, with the field oriented along all three crystallographic directions. Structural superlattice reflections at positions  $(0, \delta_m, 1)$  and  $(0, 2\delta_m, 1)$  were investigated as a function of field and temperature. For  $H||a$  and  $H||b$ , a transition from incommensurate to commensurate wave vectors is observed which coincides with the polarization flop from  $P||c$  to  $P||a$ . Whereas at zero field only second order structural superlattice reflections are observed, first order superlattice reflections appear at finite fields which are linearly increasing in intensity with the applied magnetic field. This suggests that the quadratic magneto-elastic coupling breaks down with applied magnetic field and linear magneto-elastic coupling is induced.

MA 5.3 Mon 10:45 HSZ 403

**Phase diagram of the multiferroic GdMnO<sub>3</sub> studied by thermal expansion and magnetostriction** — ●J. BAIER<sup>1</sup>, D. MEIER<sup>1</sup>, V. IVANOV<sup>2</sup>, A. MUKHIN<sup>2</sup>, A. BALBASHOV<sup>3</sup>, J. HEMBERGER<sup>1,4</sup>, and T. LORENZ<sup>1</sup> — <sup>1</sup>II. Phys. Institut, University of Cologne, Germany — <sup>2</sup>General Physics Institute, Russian Academy of Sciences, Moscow, Russia — <sup>3</sup>Moscow Power Engineering Institute, Moscow, Russia — <sup>4</sup>Institut f. Physik, University of Augsburg, Germany

Recently, the discovery of very large magnetoelectric effects in rare earth manganites  $RMnO_3$  has reopened the field of the so called multiferroic materials [1]. We present a study of the phase diagram of multiferroic GdMnO<sub>3</sub> by thermal expansion  $\alpha(T, H)$  and magnetostriction  $\epsilon(H, T)$ . GdMnO<sub>3</sub> shows an incommensurate antiferromagnetic order (ICAFM) below  $T_N \simeq 43$ K. Further decrease of temperature leads to a canted A-type antiferromagnetic ordering (cAFM) below  $T_{\text{lock}} \simeq 23$ K. Above a critical magnetic field along the  $b$  direction ferroelectric order (FE,  $P||a$ ) emerges below  $T_c \simeq 10$ K [1]. In zero magnetic field, we already observe an anomalous and anisotropic thermal expansion, but upon applying a magnetic field, very strong, new anomalies arise at the cAFM and ferroelectric phase boundary. Both phase transitions are of first-order type and display a very strong hysteresis. Furthermore we observe a down-bending of the ICAFM-to-cAFM boundary ( $T_{\text{lock}}$ ) at low magnetic fields.

[1] T. Kimura *et al.*, Nature **426**, 55 (2003), T. Kimura *et al.*, PRB **71**, 224425 (2005)

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MA 5.4 Mon 11:00 HSZ 403

**Elastomagnetic coupling of the ferrimagnetic semiconductor FeCr<sub>2</sub>S<sub>4</sub> studied with surface acoustic waves** — ●CLAUS MÜLLER<sup>1</sup>, VEACESLAV ZESTREA<sup>2</sup>, VLADIMIR TSURKAN<sup>1,2</sup>, SIEGFRIED HORN<sup>1</sup>, REINHARD TIDECKS<sup>1</sup>, and ACHIM WIXFORTH<sup>1</sup> — <sup>1</sup>Institut für Physik, Universität Augsburg, D-86159, Augsburg, Germany — <sup>2</sup>Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028, Chisinau, R. Moldova

A thin single crystalline plate of the ferrimagnetic semiconductor FeCr<sub>2</sub>S<sub>4</sub> was attached to the sound path of a surface acoustic wave (SAW) delay line. We investigated the attenuation and frequency tracking of the probing SAW in the temperature range from 4.2K to 200K. The same anomalies as in low-field magnetization measurements were seen. Since there is no coincidence of these anomalies with changes of the sheet conductance, they are related to structural transformations.

MA 5.5 Mon 11:15 HSZ 403

**Complex Magnetic Ordering Process in the Frustrated A-Site Thiospinel MnSc<sub>2</sub>S<sub>4</sub>** — ●M. MÜCKSCH<sup>1,2</sup>, A. KRIMMEL<sup>1</sup>, A. PODLESNYAK<sup>3</sup>, D. SHEPTYAKOV<sup>3</sup>, A. CERVELLINO<sup>3</sup>, V. TSURKAN<sup>1,4</sup>, C. RITTER<sup>2</sup>, M.M. KOZA<sup>2</sup>, H. MÜTKA<sup>2</sup>, S. HORN<sup>1</sup>, and A. LOIDL<sup>1</sup> — <sup>1</sup>Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — <sup>2</sup>Institut Laue-Langevin, BP 156 X, F-38042 Grenoble, France — <sup>3</sup>Laboratory for Neutron Scattering, ETHZ & PSI, CH-5232 Villigen PSI, Switzerland — <sup>4</sup>Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chisinau, Moldova

Extensive neutron scattering experiments have been performed to study the frustration effects in the magnetic A-site sulphur spinel compound MnSc<sub>2</sub>S<sub>4</sub>. Starting from the paramagnetic state above 23K a crossover to a fluctuating spin liquid phase is observed for  $T \leq 23$ K  $\approx |\theta_{CW}|$ . Approaching the magnetic ordering temperature at  $T_{N2} = 2.3$ K we discovered a broad double peak structure of the magnetic intensity around  $Q$ -positions corresponding to the  $(0.75, 0.75, 0)$  and  $(1, 0, 0)$  reciprocal lattice positions, respectively. On further cooling, for  $1.9$ K  $= T_{N1} \leq T \leq T_{N2} = 2.3$ K the peak at  $(0.75, 0.75, 0)$  sharpens and becomes dominant in intensity, whereas the intensity centered around  $(1, 0, 0)$  remains broad before completely vanishing at  $T_{N1} = 1.9$ K. This behaviour can be interpreted as a lock-in transition from an incommensurate to a commensurate structure with decreasing temperature at  $T_{N1}$ . The ground state magnetic structure of MnSc<sub>2</sub>S<sub>4</sub> is a cycloid within the  $(a, b)$ -plane characterised by a propagation vector  $\mathbf{q} \approx (0.75, 0.75, 0)$ . Below  $T_{N1}$  well defined dispersive spin-wave excitations emerge.

MA 5.6 Mon 11:30 HSZ 403

**LDA+U Picture of the Moment and Volume Collapse under Pressure in MnO** — ●DEEPA KASINATHAN<sup>1</sup>, JAN KUNES<sup>1</sup>, KLAUS KOEPERNIK<sup>2</sup>, and WARREN PICKETT<sup>1</sup> — <sup>1</sup>University of California, Davis, CA 95616 — <sup>2</sup>IFW Dresden, P.O.Box 270116, D-01171, Dresden, Germany

The transition metal monoxide MnO crystallizes in the rock-salt structure and is a high-spin antiferromagnetic insulator at low temperatures. Under pressure, experimentally it is observed to undergo a metal-insulator transition after a structural change to the nickel arsenide phase. As the first step in a concerted effort to obtain a realistic theory of the pressure behavior of MnO, we have performed full potential local orbital (FPLO) LDA+U calculations in the rock-salt phase. Within the rocksalt phase we obtain a first order moment and volume collapse at specific volume  $V/V_0 \approx 0.61$ , very close to the experimental volume. The moment collapse is from high spin state 5/2 to a low spin state 1/2, along with a 8% decrease in volume. The magnetic transition is mainly governed by the oxygen coordination. The strong influence of symmetry-lowering (cubic to rhombohedral) by antiferromagnetism is noticed with the single occupancy of the five 3d orbitals before and after collapse (*i.e.* total  $L = 0$ ). Calculations in the high pressure regime shows that the system stabilizes in the antiferromagnetic NiAs structure, in par with the observed experimental results.

MA 5.7 Mon 11:45 HSZ 403

**Orbital polarization and the metal-insulator transition in Ti2O3** — •CHUN-FU CHANG<sup>1</sup>, HOLGER OTT<sup>1</sup>, ZHIWEI HU<sup>1</sup>, MAURITS W. HAVERKORT<sup>1</sup>, HUA WU<sup>1</sup>, H. H. HSIEH<sup>2</sup>, H. -J LIN<sup>3</sup>, C. T. CHEN<sup>3</sup>, and LIU HAO TJENG<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln, Germany — <sup>2</sup>Chung Cheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan — <sup>3</sup>National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30076, Taiwan

Ti2O3 undergoes a broad metal-insulator transition (MIT) at around 400-600 K without a change in the symmetry of the corundum structure. There is a long-standing debate about the mechanism of this unusual MIT. We have set out to do polarization-dependent x-ray absorption spectroscopy measurements and cluster calculations using the configuration interaction model. We have found that the dimer effect of the vertical Ti-Ti pairs play a crucial role in the MIT. Our results point out that a gradual change of the orbital occupation of the Ti 3d states accompanies this abnormally broad transition. This orbital redistribution assists the MIT in a manner that the intersite exchange interaction of Ti-Ti pair is reduced and the effective in-plane band widths of the Ti 3d states are increased.

MA 5.8 Mon 12:00 HSZ 403

**Orbital ordering and spin gap in ruthenate La4Ru2O10** — •HUA WU<sup>1</sup>, T. BURNUS<sup>1</sup>, Z. HU<sup>1</sup>, J.D. DENLINGER<sup>2</sup>, L.-Y. JANG<sup>3</sup>, H.H. HSIEH<sup>4</sup>, P.G. KHALIFAH<sup>5</sup>, F. WANG<sup>6</sup>, J.W. ALLEN<sup>6</sup>, K.S. LIANG<sup>3</sup>, D.I. KHOMSKII<sup>1</sup>, and L.H. TJENG<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln, Germany — <sup>2</sup>Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — <sup>3</sup>National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30076, Taiwan — <sup>4</sup>Chung Cheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan — <sup>5</sup>Department of Chemistry, University of Massachusetts, Amherst, MA 01003, USA — <sup>6</sup>Randall Laboratory of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA

It was discovered [P. Khalifah *et al.*, Science **297**, 2237 (2002)] that La4Ru2O10 undergoes a rare 4d-orbital ordering transition below 160 K and acquires a spin gap. We study this interesting orbital-ordered spin-gap state both by x-ray absorption spectroscopy measurements and by LDA+U band calculations. Our results show that the Ru<sup>4+</sup> ions remain in the normal spin=1 state. A distinct orbital ordering is identified, which leads to a significant anisotropy of antiferromagnetic exchange couplings. As a result, the spin gap is opened due to formation of the Ru<sup>4+</sup>-Ru<sup>4+</sup> spin-singlet dimers but not to the originally assumed spin-state transition. Thus, La4Ru2O10 appears to be a novel orbital-ordering-assisted spin-ladder material.

MA 5.9 Mon 12:15 HSZ 403

**Magneto-optical Anisotropy of UPtGe** — •M. MARUTZKY<sup>1</sup>, J. SCHOENES<sup>1</sup>, and R. TROC<sup>2</sup> — <sup>1</sup>Institut für Physik der Kondensierten Materie und Hochmagnetfeldanlage, TU Braunschweig, Mendelssohnstr. 3, D-38106 Braunschweig — <sup>2</sup>Institute for Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50-950 Wrocław, Poland

UPtGe crystallizes in an orthorhombic EuAuGe structure. It has an incommensurable helical spin structure with  $T_N = 50$  K and two uranium sites with different magnetic moments. The magnetic and electrical properties of UPtGe are anisotropic [2]. Thereby the temperature dependence of the magnetization is similar along the *a*- and the *c*-direction, while *b* is the magnetic hard axis. Also the electrical properties are similar for *a* and *c* and different for *b*. The optical conductivity is anisotropic and merges in the dc-conductivity [3].

In this contribution the polar Kerr-rotation and -ellipticity from 1 to 4 eV of UPtGe single crystals near  $T_N$  at 12 T are presented, with various orientations of the crystal axes relative to the magnetic field and the polarization vector of the light. The Kerr-spectra are affected by the magnetic and optical anisotropy and exhibit rotations up to 0.15°. The off-diagonal elements of the optical conductivity are calculated in order to discuss the electronic structure of UPtGe.

[1] D. Mannix *et al.*, Phys. Rev. B **62**, 3801 (2000)[2] R. Troc *et al.*, Phys. Rev. B **69**, 094422 (2004)[3] M. Marutzky *et al.*, to be published

MA 5.10 Mon 12:30 HSZ 403

**An NMR analysis of magnetically ordered RMn6Ge6-xGax-compounds** — •JENS SCHNELZER, RICHARD MONTBRUN, and ELMAR DORMANN — Physikalisches Institut, Universität Karlsruhe (TH), D-76131 Karlsruhe

The  $RMn_6Ge_{6-x}Ga_x$ -compounds (R: Rare earth element) crystallize in the  $HfFe_6Ge_6$ -type structure, in which the Mn-sites are located in ferromagnetic Kagomé-nets. The R and the three inequivalent Ge-sites are arranged in hexagonal lattice sites. The influence of the variable Ga-proportion on the type of magnetic order is known and that on the NMR spectra are examined here. Spectra obtained by Nuclear Magnetic Resonance, showing zero-field <sup>73</sup>Ge, <sup>55</sup>Mn and <sup>69,71</sup>Ga resonance positions, as well as the rf-power dependent behavior, will be presented for R=Lu,Tm,Er and Ho. They can be related to the x-dependent varying magnetic structure of these compounds.

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MA 5.11 Mon 12:45 HSZ 403

**Skyrmionic textures in chiral magnets** — •U.K. RÖSSLER<sup>1</sup>, A.N. BOGDANOV<sup>1</sup>, and C. PFLEIDERER<sup>2</sup> — <sup>1</sup>IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — <sup>2</sup>Physik Department E21, TU München, Germany

In certain non-linear field models particle-like localized states, so-called Skyrmions, can be stabilized. In condensed matter systems, Skyrmions and extended Skyrmionic textures exist, e.g., under non-equilibrium conditions in turbulent fluids, induced by external fields in Quantum Hall magnets, or stabilized by topological defects in the blue phases of liquid crystals. The talk presents new theoretical results on Skyrmionic magnetization structures in magnets with broken inversion symmetry. In these chiral systems, a particular exchange, so-called Dzyaloshinskii-Moriya interactions, stabilize vortex-like Skyrmions as string-like excitations and condensates of Skyrmions with the appearance of multiply modulated states. In phenomenological models for weakly ferromagnetic metals, Skyrmion lattices spontaneously arise as equilibrium phases. The theory explains the "partial magnetic order", recently found in the chiral ferromagnet MnSi, as a Skyrmionic texture. Magnetic Skyrmion lattices are predicted to exist quite generally in magnetic metal films owing to the broken inversion symmetry at surfaces.