KR 1: Multiferroics I (Joint Session of MA, DF, DS, KR, TT)

Time: Monday 14:45–17:00 Location: HSZ 04

KR 1.1 Mon 14:45 HSZ 04

DFT calculation of $ACrO_3$ perovskites using hybrid functionals — •Martin Schlipf[1], Alessandro Stroppa[2], Silvia Picozzi[2], and Marjana Ležaić[1] — [1]Forschungszentrum Jülich, Peter Grünberg Institut and JARA, Germany — [2]CNR-SPIN, L'Aquila, Italy

Density-functional theory (DFT) is a very powerful tool for understanding the properties of several crystals and molecules. Novel hybrid exchange-correlation functionals, which include a fraction of Hartree-Fock exchange, improved the predictive power of DFT further. In this contribution, we have studied the $ACrO_3$ (A = Ca, Sr, Pb) perovskite compounds by DFT. These materials have recently gained a renewed interest, because they offer a rich phase-space of electronic, magnetic and structural transitions. The origins of several of these transitions are not understood, yet. In $SrCrO_3$ different authors report different electronic (metal/insulator) and magnetic (Pauli paramagnetic/Curie Weiss) configurations. It is not clear yet what is the ground state of this compound. In $PbCrO_3$ theoretical calculations predict a conducting state whereas experimentally a metal is found. We use a multi-code approach and clarify these issues from first-principles.

We gratefully acknowledge the support from HGF Nachwuchsgruppe Programme VH-NG-409.

KR 1.2 Mon 15:00 HSZ 04

Optical properties of $BiCrO_3$ — •Cameliu Himcinschi[1], Ionela Vrejoiu[2], Silvia Bahmann[1], Kannan Vijayanandhini[2], Adreas Talkenberger[1], Christian Röder[1], Dietrich R.T. Zahn[3], Alexei A. Belik[4], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, D-06120 Halle — [3]TU Chemnitz, Semiconductor Physics, D-09107 Chemnitz — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

Multiferroic materials that simultaneously show polarization and magnetization ordering are envisaged to play a significant role in developing devices with large magnetoelectric coupling. An interesting candidate for intrinsic multiferroism is $BiCrO_3$ (BCO). In this work, the optical properties of polycrystalline BCO ceramics and epitaxial BCO films deposited on $NdGaO_3$(110) substrates are investigated by Raman spectroscopy and spectroscopic ellipsometry. The spectral changes seen in temperature-dependent Raman measurements correlate well to a structural phase transition from a monoclinic structure (space group *C2/c*) to an orthorhombic structure (space group *Pnma*) at about 420 K. The room temperature dielectric function of a 55 nm thick BCO film deposited on $NdGaO_3$ substrate is determined by analyzing ellipsometry data and exploited to estimate the BCO band-gap. The imaginary part of the dielectric function calculated by means of density functional theory shows good agreement with the experimental one. *This work was supported by the German Research Foundation DFG HI 1534/1-1.*

KR 1.3 Mon 15:15 HSZ 04

Pressure induced phase transitions in $MnTiO_3$: Insights from First Principles calculations — •Carmen Quiroga and Rossitza Pentcheva — Section Crystallography, Dept. of Earth and Environmental Sciences, University of Munich

$MnTiO_3$ crystallizes in the ilmenite structure at ambient conditions and remains stable at least up to 26 GPa [1]. A denser $LiNbO_3$ phase can be quenched from high pressure and high temperature experiments to ambient conditions [2]. Our density functional theory calculations, including an on-site Coulomb repulsion term (LDA/GGA+U), show a transition from the $LiNbO_3$ to the perovskite phase at 2.5 GPa in agreement with experiments [3]. A transition from perovskite to the post-perovskite phase ($CaIrO_3$-type) is predicted at pressures above 50 GPa. Furthermore, the magnetic coupling of the Mn ions and the possibility of spin transitions in the different phases are explored.

Funding by DFG SPP1236 (PE883/8-1) is acknowledged.

[1] X. Wu et al. Geoscience Frontiers, in press (2010).
[2] J. Ko and C.T. Prewitt. Phys. Chem. Minerals **15**, 355 (1988).
[3] N. Ross et al. Phys Chem Minerals **16**, 621 (1989).

KR 1.4 Mon 15:30 HSZ 04

Resonant Soft X-ray Scattering (RSXS) Studies on Multiferroic YMn2O5 — •Sven Partzsch[1], Stuart Wilkins[2], John Hill[2], Enrico Schierle[3], Eugen Weschke[3], Dmitri Souptel[1], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW Dresden — [2]BNL Upton — [3]Helmholz-Zentrum Berlin

Multiferroic RMn_2O_5 (R = Y, rare earth, Bi) displays a complex magnetic behavior with transition into a ferroelctric phase as a function of temperature. The intensity of the magnetic superlattice reflection $(1/2, 0, 1/4)$ displays a strong resonance at the Mn L_{23}-edge, due to the strongly increased magnetic sensitivity close to the absorption edge.

Surprisingly, we also observe that this magnetic peak also displays a strong resonance at the oxygen K-edge. The measured integrated intensity of this reflection at the Mn L_3-edge in the commensurate and incommensurate magnetic phase is essentially unchanged. At the oxygen K-edge, however, a strong drop of the temperature dependent integrated intensity is observed at the corresponding phase transition, which resembles the temperature dependence of the ferroelectric polarization. Therefore RSXS at the different edges might provide more information about the origin of ferroelectricity in these frustrated magnets.

The experimental data together with LSDA+U calculations provide evidence that magnetically driven charge transfer between oxygen and manganese plays an important role for the ferroelectricity in these frustrated magnets.

KR 1.5 Mon 15:45 HSZ 04

Dilatometric studies of the multiferroic $FeTe_2O_5Br$ — •Christian Balz[1], Mariano de Souza[1], Matej Pregelj[2], Helmuth Berger[3], Denis Arčon[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt(M), SFB/TR49, Germany — [2]Institute "Jozef Stefan", Jamova 39, 1000 Ljubljana, Slovenia — [3]Institute of Physics of Complex Matter, EPFL, 1015 Lausanne, Switzerland

We report on high-resolution directional dependent thermal expansion measurements of the novel multiferroic system $FeTe_2O_5Br$ [1]. Our results reveal two distinct phase transition anomalies centered at $T_{N1} = 11.0$ K and $T_{N2} = 10.6$ K, which coincide with the transitions observed in other quantities [2]. A rounded minimum in α_c shows that short-range magnetic correlations within the crystal layers start to develop already above T_N. At T_{N1}, the system undergoes a magnetic phase transition into the high-T incommensurate (HT-ICM) phase. Interestingly, at T_{N2}, a second phase transition into the low-T incommensurately modulated (LT-ICM) phase is observed, which is accompanied by a spontaneous electric polarization. When magnetic field is applied, the transition temperatures shift depending on the field orientation. In the case of $B \| b > 4.5$ T, the HT-ICM phase merges into the LT-ICM phase. Despite the pronounced lattice effects observed at T_{N2} at 6 T, the electric polarization is destroyed. The rich low-T magnetic phase diagram of $FeTe_2O_5Br$ will be discussed in details [2].

[1] M. Pregelj *et al.*, Phys. Rev. Lett. **103**, 147202 (2009).
[2] M. Pregelj *et al.*, Phys. Rev. B **82**, 144438 (2010).

KR 1.6 Mon 16:00 HSZ 04

Investigation of multiferroic order in M_3TeO_6 (M=Co, Mn, Ni) by second harmonic generation — •Vera Carolus[1], Thomas Lottermoser[1], Sergey A. Ivanov[2], Matthias Weil[3], Roland Mathieu[4], Matthias Hudl[4], Per Nordblad[4], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]Department of Inorganic Materials, Karpov' Institute of Physical Chemistry, Vorontsovo pole, 10 105064, Moscow K-64, Russia — [3]Institute of Chemical Technologies and Analytics, Vienna University of Technology, Austria — [4]Department of Engineering Sciences, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden

Orthotellurates with the formula M_3TeO_6 are structurally well characterized and can be divided into six different structure types. According to this, these materials show a wide range of magnetic phases. Recently it was suggested, that in some of the orthotellurates multiferroic order is possible.

Among this are: Co_3TeO_6 (space group C2/c) and Mn_3TeO_6 ($R\bar{3}$) with two magnetic phase transitions as well as Ni_3TeO_6 (R3) with one magnetic phase transition. However, a direct proof of ferroelectricity has not been reported so far.

Here, we investigate the multiferroic order by second harmonic generation (SHG) spectroscopy. For Co_3TeO_6 we measured a intense SHG contribution in the low temperature phase below 18 K, which is a strong evidence for multiferroic order. This interpretation is supported by the observation of complex domain patterns using SHG imaging techniques.

KR 1.7 Mon 16:15 HSZ 04

Optical Spectroscopy on the triangular antiferromagnet $CuCrO_2$ — •Michael Schmidt, Zhe Wang, Franz Mayr, Vladimir Tsurkan, Joachim Deisenhofer, and Alois Loidl — Experimental Physics 5, Center for Electronic Correlations and Magnetism, Institute of physics, Augsburg University, Germany

$CuCrO_2$ belongs to the class of triangular lattice antiferromagnets and shows ferroelectricity below $T_{FE} \approx 24$ K [1] while the spins order in a proper screw [2]. Already a moderate magnetic field of 5.3 T can flop the plane of the spins and the polarization. A microscopic theory [3] explains this by the variation of the spin-orbit coupling with the metal-ligand (d-p) hybridization. Recently, electromagnons (magnetic excitations excited by electric field) have been detected in the related compound $Cu(Fe,Al)O_2$ [4] in the submillimeter range. We report on the optical excitation spectrum of $CuCrO_2$ including phonons, crystal-field excitations and magnon sidebands. The relation of magnon lifetime with the possible formation of Z_2 vortices in this system is discussed.

[1] K. Kimura et al., Phys. Rev. B 78, 140401 (2008)
[2] S. Seki et al., Phys. Rev. Lett. 101, 067204 (2008)
[3] T. Arima J. Phys. Soc. Jap. 76, 073702 (2007)
[4] S. Seki et al., Phys. Rev. Lett. 105, 097207 (2010)

KR 1.8 Mon 16:30 HSZ 04

New design for magnetoelectric switch from first principles — •Michael Fechner[1], Peter Zahn[2], Sergey Ostanin[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik Halle, Germany — [2]Fachgruppe Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg

Saving information in a magnetic bit requires at least two stable magnetic states that can be distinguished. In conventional hard disks two opposite directions of the magnetization provide these two states. The magnetic state is changed by an external magnetic field thus writing information, whereas reading is performed by the usage of the GMR effect (giant magnetoresistance) [1]. Based on ab intio material design we propose a new hybrid magnetoelectric that allows this switching of the magnetic states by an applied electric field instead of the magnetic field. The switching in the proposed multilayer system is based on internal electronic couplings without any strain. Thus, it is a promising candidate for application in future magnetoresistive random access memory (MRAM).

[1] Baibich et al., PRL 61, 2472-2475, (1988)

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