

DF 5: Multiferroics II (Joint Session of MA, DF, KR, DS)

Time: Monday 14:00–17:45

Location: H3

DF 5.1 Mon 14:00 H3

Switching of a spin-spiral-induced polarization in multiferroic MnWO₄ — ●TIM HOFFMANN¹, DENNIS MEIER¹, PETRA BECKER-BOHATÝ², LADISLAV BOHATÝ², and MANFRED FIEBIG¹ — ¹HISKP, Universität Bonn — ²Institut für Kristallographie, Universität zu Köln

Coexisting ferroic orders become interesting when there is an interaction between them. Especially applying an electric field and thus changing the magnetic order is highly desirable for possible applications. In spite of the declared interest in multiferroics to switch a magnetization by an electric field nothing is known about the dynamics of the actual switching process.

The coupling of ferroelectric and magnetic order is intrinsically strong in spin-spiral multiferroics, where ferroelectricity emerges as a consequence of complex magnetic long-range order. Here we observe the manipulation of magnetically-induced ferroelectric domains in MnWO₄ by optical second harmonic generation (SHG). Application of an electric field allows to transform the sample to an electric as well as magnetic single-domain state. Moreover we obtained images of the domain structures during the transition revealing the growth of the domains. When cooled in zero-field, the domains have a bubble-like topology. Interestingly, after recovery from a single domain state the shape changes to a stripe structure and the domain size is significantly increased. Effects of the shape and duration of the electric-field poling pulses are investigated. Furthermore, in contrast to typical ionic ferroelectrics the spontaneous polarization can be switched without fatigue – no defects or pinning effects constrain the movement of domain walls.

DF 5.2 Mon 14:15 H3

Single Crystal X-ray diffraction studies on multiferroic YMn_{2-x}Fe_xO₅ — ●SVEN PARTZSCH¹, JOCHEN GECK¹, NORMAN LEPS¹, ROBERTO KRAUS¹, DMITR SOUPEL¹, BERND BÜCHNER¹, and ENRICO SCHIERLE² — ¹IFW Dresden — ²Helmholz-Zentrum Berlin

Temperature dependent single crystal X-ray diffraction studies of YMn_{2-x}Fe_xO₅ are presented. Upon cooling, the undoped material (x=0) orders antiferromagnetically below $T_N \approx 45$ K and becomes multiferroic below $T_{CE} \approx 39$ K. This multiferroic phase is destabilized rapidly with increasing Fe-content and we address here the reasons for this dramatic effect. The crystallographic study implies that the doped Fe mainly occupies the square pyramidal coordinated Mn position instead the octahedral one, which shows that these lattice sites are crucial for the MF properties.

In order to further characterize the electronic ordering in the ferroelectric phase of the undoped samples, we also applied soft resonant X-ray diffraction, which clearly shows that the oxygen states play an important role as well.

DF 5.3 Mon 14:30 H3

Electronic structure and magnetism in YFeMnO₅ — ●TORSTEN WEISSBACH¹, TILMANN LEISEGANG², AXEL LUBK², DIRK C. MEYER³, and SIBYLLE GEMMING⁴ — ¹Inst. f. Theoretische Physik, TU Bergakademie Freiberg — ²Inst. f. Strukturphysik, TU Dresden — ³Inst. f. Experimentelle Physik, TU Bergakademie Freiberg — ⁴Inst. f. Ionenstrahlphysik u. Materialforschung, Forschungszentrum Dresden

YFeMnO₅ crystallizes in the structure type of the orthorhombic $R\text{Mn}_2\text{O}_5$ class of oxides. These show a series of antiferromagnetic phases with propagation vectors $(1/2-\delta, 0, 1/4+\epsilon)$ below $T_N \approx 45$ K. For several of these phases, magnetism coexists with ferroelectricity. In YFeMnO₅, only one commensurable ferrimagnetic phase was found below $T_N = 165$ K, and ferroelectricity is absent. We apply crystallographic and quantum chemical methods to compare the Fe-substituted and the manganese-only compounds. Diffraction experiments show slight displacements of the atom sites with increasing Fe content. The largest effects are related to crystal-field repulsion acting on the local metal 3d orbitals. The interaction between the magnetic metal ions is studied using DFT calculations starting with a bias magnetization of the atoms.

DF 5.4 Mon 14:45 H3

Ab initio calculations of the magnetic properties of perovskites under deformation — ●IGOR MAZNICHENKO¹, CORINA ETZ², ARTHUR ERNST², MARTIN LÜDERS³, INGRID MERTIG^{1,2}, ZDZIS-

LAWA SZOTEK³, and WALTER TEMMERMAN³ — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — ²Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany — ³Daresbury Laboratory, Daresbury, Warrington WA4 4AD, Cheshire, United Kingdom

Materials with perovskite and perovskite-like structures demonstrate a broad spectrum of physical properties. Colossal magnetoresistance, ferroelectricity, multiferroicity, superconductivity, charge ordering, metal-insulator transition, Jahn-Teller and other effects are observed in perovskites. These properties of the mentioned materials with the common formula ABO_3 are very sensitive to the type of the cations A and B . $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ (LSMO) is a strongly correlated 3d transition metal oxide with a Curie temperature (T_C) above RT (370 K). For other La/Sr ratios different types of antiferromagnetism are observed. Other perovskite, ruthenate SrRuO_3 (SRO) is a 4d ferromagnet with $T_C = 160$ K.

Here we perform *ab initio* calculations for LSMO and SRO in ideal cubic, tetragonally distorted, and different orthorhombic structures. We focus on magnetic order and Curie temperature of the above mentioned structures in the different structural phases.

DF 5.5 Mon 15:00 H3

Electric field induced magnetization switching in strained EuO — ●MARJANA LEŽAIĆ, KONSTANTIN RUSHCHANSKII, FRANK FREIMUTH, and STEFAN BLÜGEL — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

EuO is one of the rare materials combining a semiconducting gap and ferromagnetic ordering. Due to this property, EuO was suggested as a spin-filter in magnetic tunnel junctions [1]. It was shown that its ordering temperature T_C of 69 K can be increased further by doping with Gd [2], or by a reduction of the lattice parameter [3]. Recently, it has also been shown that a spin-polarized 2-dimensional electron gas can be formed at the EuO/LaAlO₃ interface [4]. The list of properties that are not only interesting from the point of view of basic research, but also indicate possible applications, does not end here. A newly discovered property, ferroelectricity in strained EuO [5] puts this material into the class of multiferroics with relatively high T_C . Employing *ab-initio* calculations, we demonstrate how the ferroelectric property can be exploited in EuO films under tensile strain in order to achieve electric control of the magnetization direction.

- [1] T. Santos and J. S. Moodera, Phys. Rev. B **69**, 241203 (2004).
- [2] R. Sutarto, *et al*, Phys. Rev. B **80**, 085308 (2009).
- [3] N. J. C. Ingle and I. S. Elfimov, Phys. Rev. B **77**, 121202(R) (2008).
- [4] Y. Wang, *et al*, Phys. Rev. B **79**, 212408 (2009).
- [5] E. Bousquet, N. A. Spaldin, Ph. Ghosez, arXiv:0906.4235v1.

DF 5.6 Mon 15:15 H3

Ferroelectric properties of BiFeO₃ thin films under mechanical stress — ●MARTIN HOFFMANN, OLIVER MIETH, and LUKAS M. ENG — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Since ferroelectric properties (polarization, coercive field, etc.) of thin films can differ dramatically from the corresponding bulk values due to lattice-mismatch-induced strain, the systematic investigation of the impact of mechanical stress on the nm-length-scale is an indispensable step towards the general understanding of ferroic thin film physics.

In the present study, 150-nm-thick multiferroic BiFeO₃ films grown on (001)-oriented SrTiO₃ substrates were inspected with piezoresponse force microscopy (PFM) towards their ferroelectric domain distribution and their local ferroelectric hysteresis behavior under both tensile and compressive stress.

The systematic variation of the externally applied mechanical stress by substrate bending allowed us to compensate or to enhance the strain effect, which can be quantified by monitoring the coercive field as a function of the bending angle.

DF 5.7 Mon 15:30 H3

Strain effects in spinel ferrite thin films from first principles calculations — ●DANIEL FRITSCH and CLAUDE EDERER — School of Physics, Trinity College Dublin, Ireland

We present density functional theory calculations of the structural and magnetic properties of the inverse spinel systems CoFe_2O_4 (CFO) and NiFe_2O_4 (NFO). Both are insulating magnets with high magnetic ordering temperatures and large saturation magnetization, which have been of particular interest over the past few years as building blocks of multiferroic heterostructures [1]. In order to effectively design the magneto-electric response of such multiferroic heterostructures, a clear picture of strain-induced changes in the magnetic properties of CFO and NFO is particularly important. Here we present results for the structural and magnetic properties of both CFO and NFO, with special emphasis on strain-induced changes in the magneto-crystalline anisotropy energy (MAE). Our results are representative for (001)-oriented thin films of CFO and NFO, grown on different lattice-mismatched substrates. We find a large and strongly strain-dependent MAE for CFO, and a significantly smaller but also strongly strain-dependent MAE for NFO. We discuss the influence of cation order within the inverse spinel structure and analyze the effect of different exchange correlation functionals on the structural and magnetic properties.

[1] H. Zheng et al., *Science* 303, 661 (2004).

15 min. break

DF 5.8 Mon 16:00 H3

Mechanism of ferroelectric instabilities in non-d⁰ perovskites: LaCrO_3 versus CaMnO_3 — TIM HARRIS, ROMAN KOVACIK, and •CLAUDE EDERER — School of Physics, Trinity College Dublin, Ireland

The incompatibility of partial d occupation on the perovskite B -site with the standard charge transfer mechanism for ferroelectricity has been a central paradigm in multiferroics research [1]. Nevertheless, it was recently shown by density functional theory calculations that CaMnO_3 exhibits a polar instability that even dominates over the octahedral tilting for slightly enlarged unit cell volume [2]. Here, we present similar calculations for LaCrO_3 , which has the same d^3 B -site electron configuration as CaMnO_3 . We show that LaCrO_3 exhibits a similar, albeit somewhat weaker, volume-dependent polar instability as CaMnO_3 , but while the Born effective charge (BEC) for the Mn^{4+} cation in CaMnO_3 is highly anomalous, the BEC for Cr^{3+} in LaCrO_3 is only slightly enhanced. We decompose the BECs for both systems in contributions of individual Wannier functions to elucidate the different driving force behind the polar instability in these systems.

[1] N. A. Hill, *J. Phys. Chem. B* 104, 6694 (2000). [2] S. Bhatnagar et al., *Phys. Rev. Lett.* 102, 117602 (2009).

DF 5.9 Mon 16:15 H3

Multiferroicity in EuTiO_3 and $\text{Eu}_{1-x}\text{Ba}_x\text{TiO}_3$: *ab initio* characterization of crystalline, magnetic and electronic structure — •KONSTANTIN Z. RUSHCHANSKII¹, MARJANA LEŽAIC¹, and NICOLA A. SPALDIN² — ¹Institut für Festkörperforschung, Quanten-Theorie der Materialien, Forschungszentrum Jülich GmbH, 52425 Jülich, and JARA-FIT, Germany — ²Materials Department, University of California, Santa Barbara, CA 93106-5050, USA

We report a systematic study of possible structural transitions in EuTiO_3 and ordered $\text{Eu}_{1-x}\text{Ba}_x\text{TiO}_3$ mixed compounds. We investigated phonon spectra of EuTiO_3 and found strong M- and R-point instabilities, indicating antiferrodistortive structural deformations. In the ordered $\text{Eu}_{0.5}\text{Ba}_{0.5}\text{TiO}_3$ compounds, the antiferrodistortive deformation is replaced by significant ferroelectric distortions, involving not only Ti, but also the magnetic Eu cation. We will discuss several scenarios of ferroelectric and antiferrodistortive transitions and their coupling with the magnetic structure. Corresponding changes in the phonon structure will be compared with available experimental data.

DF 5.10 Mon 16:30 H3

Electronic and magnetic properties of LuFe_2O_4 — •KARSTEN KUEPPER¹, MICHAEL RAEKERS², CHRISTIAN TAUBITZ², MANUEL PRINZ², CHRISTINE DERKS², MANFRED NEUMANN², ANDREI V. POSTNIKOV³, FRANK M. F. DE GROOT⁴, CINTHIA PIAMONTEZE⁵, DHARMALINGAM PRABHAKARAN⁶, and STEPHEN J. BLUNDELL⁶ — ¹Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm, Germany — ²Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — ³LPMD, Paul Verlaine University and Institute Jean Barriol, Metz, France — ⁴Department of Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan 16, 3584 CA Utrecht, Netherlands — ⁵Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

— ⁶Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, United Kingdom

LuFe_2O_4 is a compound showing fascinating magneto electric coupling via charge ordering. Electronic and magnetic properties of the charge ordered phase of LuFe_2O_4 are investigated by means of x-ray spectroscopic and theoretical electronic structure approaches [1]. We identified the electronic states of the valence band by means of valence band XPS-, and XES-spectroscopies, and GGA+ U first principles calculations. Moreover, by applying XMCD, we are able to identify the spin ground state of LuFe_2O_4 in the charge ordered phase to be a 2:1 ferrimagnetic configuration, ruling out a frustrated magnetic state.

[1] K. Kuepper et al., *Phys. Rev. B, Rapid Commun.*, in press.

DF 5.11 Mon 16:45 H3

Influence of Fe-substitution in $\text{LiNi}_{(1-x)}\text{Fe}_x\text{PO}_4$ on the antiferromagnetic structure — •ELKE KÜNZEL¹, ANNE ZIMMERMANN¹, JIYING LI², DAVID VAKNIN², and MANFRED FIEBIG¹ — ¹HISKP, Universität Bonn — ²Ames Laboratory and Department of Physics, Iowa States University, Ames, USA

The LiMPO_4 system ($M=\text{Fe, Ni, Co, Mn}$) includes crystallographically isostructural compounds with antiferromagnetic (AFM) order differing in the spin direction only. Thus, the system offers the opportunity to study fundamental mechanisms of AFM 180° domain formation in a range of similar but not identical compounds. In spite of their structural similarity, drastic differences in the domain topology are observed by optical SHG. Domains in LiNiPO_4 form anisotropic platelets whereas in LiFePO_4 they are isotropic and amoeba-like. It is yet unclear whether this surprising behaviour is due to the properties of the nickel ion or to the spin direction which points along z in LiNiPO_4 and along y in LiFePO_4 .

In order to clarify this, samples with different mixing ratios of nickel and iron were studied. The domain structure of LiNiPO_4 was found to become amoeba-like for an iron substitution of «50%. An anomalous temperature dependence of the AFM order parameter and indications for a spin structure different from that of the end compounds was observed.

DF 5.12 Mon 17:00 H3

Non-Resonant Magnetic X-ray Scattering on Rare-Earth Iron Borates $\text{RFe}_3(\text{BO}_3)_4$ — •JORGE E. HAMANN-BORRERO¹, MARTIN PHILIPP¹, OLGA KATAEVA², MARTIN VON ZIMMERMANN³, CHRISTIAN HESS¹, RUEDIGER KLINGELER¹, ALEXANDER VASILIEV⁴, LEONARD BEZMATERNYKH⁵, and BERND BUECHNER¹ — ¹IFW Dresden, 01171 Dresden, Germany — ²A.E.Arbutov Institute of Organic and Physical Chemistry of the Russian Academy of Sciences, Kazan, Russia — ³HASYLAB at DESY, Hamburg, Germany. — ⁴Low Temperature Physics department, Faculty of Physics, Moscow State University, Moscow, Russia. — ⁵L.V. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia.

Non-resonant magnetic XRD (NRMXRD) experiments with photon energy of 100keV where performed on selected compounds of the $\text{RFe}_3(\text{BO}_3)_4$ family as a function of temperature and applied magnetic field. The results show the existence of several unexpected diffraction features, in particular the presence of a magnetic super-lattice peak, and the appearance of two reflections that violate the diffraction conditions for the low temperature phase $P3_121$ of the iron borates. The magnetic nature of the former is concluded from analysing the scattering cross section at high energies and the magnetic structure of the different compounds. It is shown that the magnetic reflection reveals the magnetic properties of the material. For $\text{GdFe}_3(\text{BO}_3)_4$, values for the component of the spin moment perpendicular to the scattering plane (S_{\perp}) have been determined as well as the angle between the spin moment and the hexagonal basal plane.

DF 5.13 Mon 17:15 H3

Electronic structure, magnetic and dielectric properties of the edge-sharing copper-oxide chain compound NaCu_2O_2 — •PHILIPPE LEININGER¹, MARTIN RAHLENBECK¹, MARKUS RAICHEL¹, BRITTA BOHNENBUCK¹, ANDREY MALYUK², CHENGTIAN LIN¹, BERNHARD KEIMER¹, EUGEN WESCHKE², ENRICO SCHIERLE², SHINICHIRO SEKI³, YOSHI TOKURA³, and JOHN FREELAND⁴ — ¹Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin, Germany — ³University of Tokyo, Dept. of Applied Physics, Bunkyo-ku, Tokyo 113-8656, Japan — ⁴Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA

We report an experimental study of NaCu₂O₂, a Mott insulator containing chains of edge-sharing CuO₄ plaquettes, by polarized x-ray absorption spectroscopy (XAS), resonant magnetic x-ray scattering (RMXS), magnetic susceptibility, and pyroelectric current measurements. The XAS data show that the valence holes reside exclusively on the Cu²⁺ sites within the copper-oxide spin chains and populate a d-orbital polarized within the CuO₄ plaquettes. Our results also demonstrate a new orbital selection rule for RMXS that is of general relevance for magnetic structure determinations by this technique. Dielectric property measurements reveal the absence of significant ferroelectric polarization below T_N, which is in striking contrast to corresponding observations on the isostructural compound LiCu₂O₂. The results are discussed in the context of current theories of multiferroicity.

DF 5.14 Mon 17:30 H3

Magnetoelectric effect in diluted antiferromagnet PbFe_{0.5}Nb_{0.5}O₃ — •VLADIMIR SHVARTSMAN¹, PAVEL BORISOV², WOLFGANG KLEEMANN², and ANTONI KANIA³ — ¹Institut für Materialwissenschaft, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Essen, Germany — ²Angewandte Physik, Fakultät

für Physik, Universität Duisburg-Essen, Duisburg, Germany — ³Institute of Physics, University of Silesia, Katowice, Poland

Multiferroics, i. e. materials where two primary ferroic order parameters of magnetic and electric nature coexist, are of significant scientific and practical interest nowadays. Especially attractive are the multiferroics with enhanced magnetoelectric (ME) properties, which relate changes of polarization/magnetization to external magnetic/electric fields, respectively. While the linear ME effect has strong symmetry requirements and is rare, higher order ME couplings are allowed in all multiferroics. We report on investigations of magnetic and ME properties of (001)-oriented PbFe_{0.5}Nb_{0.5}O₃ (PFN) single crystals in the temperature range 5-300 K. PFN is ferroelectric below 385 K and antiferromagnetic below the Néel temperature, T_N=154 K. Temperature dependences of the magnetization exhibit a step like anomaly at T_N and a maximum on zero-field cooled curves at 8 K. Below T_N, the system manifests a spontaneous second order ME effect (electrobimagnetic effect), which reaches a peak value around 20 K. Moreover, after field cooling the linear ME effect has been observed, which disappears above 8 K. The nature of the low-temperature magnetic anomaly and the temperature dependences of the ME effects are discussed.