

TT 77: Multiferroics
(Joint session of MA, DF, DS, KR and TT organized by MA)

Time: Thursday 15:00–17:30

Location: H34

TT 77.1 Thu 15:00 H34

Skymionic and ferromagnetic resonances in magnetoelectric Cu_2OSeO_3 - magnetic vs electric fields — ●S. HARMS¹, M. BELESÍ², H. BERGER³, J.-F. ANSERMET³, C. GRAMS¹, P. BECKER¹, and J. HEMBERGER¹ — ¹University of Cologne, Germany — ²IFW, Dresden, Germany — ³ICMP, EPFL, Lausanne, Switzerland

Magnetic Skymions are topologically stable spin whirls stabilized by spin-orbit interaction in chiral cubic magnets. It has been shown, that skymionic structures can be efficiently manipulated by small forces, such as e.g. currents in metallic host materials [1]. It was also shown, that the skymion phases in general can be excited by AC magnetic fields in the microwave range. [2].

The magnetoelectric helimagnetic insulator Cu_2OSeO_3 is one of the up to now rare cases of an insulating chiral magnets showing a stable skymion lattice embedded in between helical and ferrimagnetic phases. In this compound the lack of magnetic inversion symmetry leads to the occurrence of electric polarization and correspondingly to a magnetoelectric response. We present results of broadband spectroscopy up to 5 GHz trying to disentangle the different influence of electric and magnetic fields.

Funded through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

- [1] T. Schulz et al., Nature Physics 8, 301-304 (2012).
[2] Y. Onose et al., Phys. Rev. Lett. 109, 037603 (2012).

TT 77.2 Thu 15:15 H34

Multiferroic vs. magnetoelectric properties of the dilution series $[(\text{NH}_4)_{1-x}\text{K}_x]_2[\text{FeCl}_5(\text{H}_2\text{O})]$ — ●DANIEL BRÜNING¹, MATTHIAS ACKERMANN¹, LADISLAV BOHATY², PETRA BECKER², and THOMAS LORENZ¹ — ¹II. Physikalisches Institut, Universität zu Köln, Germany — ²Institut für Kristallographie, Universität zu Köln, Germany

Recently we found that $(\text{NH}_4)_2[\text{FeCl}_5(\text{H}_2\text{O})]$, a member of the antiferromagnetic erythrosiderites $A_2[\text{FeX}_5(\text{H}_2\text{O})]$ ($A = \text{K}, \text{Rb}, \text{Cs}$ or NH_4 and $X = \text{Cl}$ or Br) is multiferroic with a spontaneous polarization at $T_C = 6.87\text{K}$, slightly below the magnetic ordering at $T_N = 7.25\text{K}$. Additionally we found a high-temperature structural phase transition $T_{st} = 79\text{K}$, related to a monoclinic distortion (Pnma to $P11_2^2$) due to a rearrangement of the hydrogen atoms. In contrast to $(\text{NH}_4)_2[\text{FeCl}_5(\text{H}_2\text{O})]$, the related erythrosiderites with $A = \text{K}, \text{Rb}$ or Cs are not multiferroic, but show linear magnetoelectric coupling with $P_i = \alpha_{ij}H_j$ below T_N . Investigating the dilution series with $A = (\text{NH}_4)_{1-x}\text{K}_x$ provides information on the stability of the multiferroic versus magnetoelectric behavior. Based on dielectric and magnetic measurements we present detailed magnetic-field versus temperature phase diagrams. Interestingly, the mixed crystals develop a finite pyroelectric polarization at T_{st} , whereas there is no indication of pyroelectricity above T_N , neither in the pure (NH_4) -based nor in the pure K-based compound.

- M. Ackermann et al., J. Phys.: Condens. Matter, **26**, 506002, (2014)
M. Ackermann et al., New J. Phys., **15** 123001, (2013)

TT 77.3 Thu 15:30 H34

Optical switching of multiferroic domains in TbMnO_3 — ●SEBASTIAN MANZ¹, MASAKAZU MATSUBARA^{1,2}, JONATHAN BÜCHI¹, THOMAS LOTTERMOSER¹, AYATO IYAMA³, TSUYOSHI KIMURA³, DENNIS MEIER¹, and MANFRED FIEBIG¹ — ¹Department of Materials, ETH Zürich, 8093 Zurich, Switzerland — ²Department of Physics, Tohoku University, Sendai 980-8578, Japan — ³Division of Materials Physics, Osaka University, Osaka 560-8531, Japan

Multiferroics with spin-spiral-driven ferroelectricity possess a strong coupling between electric and magnetic domains, rendering them interesting for future technological devices. Controlling these domains on the local scale is an essential prerequisite, e. g. for data storage applications. Current discussions on spin-spiral multiferroics, however, focused on the conversion of one domain state into the other but reversible local manipulation has not been shown yet. As presently demonstrated in ferri- and ferromagnets, all-optical switching offers a promising route to achieve localized control. Here, we demonstrate spatially-resolved optical switching of antiferromagnetism in multifer-

roic TbMnO_3 . We manipulate the antiferromagnetic order via the coupled ferroelectric state using a unique relation between the wavelength of the light and the induced polarization change. This allows us to realize reversible switching of multiferroic domains without any external bias fields. To further understand our results, we performed Monte-Carlo simulations which confirmed our findings. Our proof-of-principle experiments show that multiferroic domains and therefore domain walls can be generated and erased entirely optically on the local scale.

TT 77.4 Thu 15:45 H34

Investigation of the photostriction effect in BiFeO_3 by means of infrared and optical spectroscopy — ●FLORIAN BURKERT and CHRISTINE KUNTSCHER — Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany

It has been reported that BiFeO_3 crystals change their size during illumination with visible light or ultraviolet radiation [1,2]. We studied the impact of this photostrictive effect on the optical properties of a BiFeO_3 single crystal in the infrared up to the ultraviolet frequency range by using an FTIR spectrometer and a CCD spectrograph. During illumination with various radiation sources we observe the appearance of additional absorption features in the optical spectra. We will discuss possible origins of these new features.

- [1] B. Kundys et al., Nat. Mater. **9**, 803 (2010)
[2] B. Kundys et al., Phys. Rev. B **85**, 092301 (2012)

15 min. break

TT 77.5 Thu 16:15 H34

Epitaxial engineering of ferrimagnetic 3d-5d double perovskites as templates for single phase multiferroics — ●VIKAS SHABADI¹, ASHISH KULKARNI^{1,2}, PHILIPP KOMISSINSKIY¹, IVETTA SLIPUKHINA³, ROBERT PARIÁ SENA⁴, JOKE HADERMANN⁴, RAJEEV GUPTA², HONGBIN ZHANG¹, MARJANA LEŽAIČ³, and LAMBERT ALFF¹ — ¹Institute of Materials Science, Technische Universität Darmstadt, Germany — ²Materials Science Programme, IIT Kanpur, India — ³Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Germany — ⁴Electron Microscopy for Materials Science (EMAT), University of Antwerp, Belgium

3d-5d double perovskites ($A_2BB'O_6$) are of high interest due to the possible large magnetic ordering temperatures [1], multiferroicity, and the influence of spin-orbit coupling. We have for the first time synthesized in thin film form double perovskites with $\text{Mn}^{2+}/\text{Re}^{4+}$ and $\text{Ni}^{2+}/\text{Re}^{4+}$ cations at the B/B' -sites and La^{3+} at the A -site, previously predicted by density functional theory (DFT). We have shown the almost perfect ordering at the B -site by X-ray diffraction and high-angle annular dark field scanning transmission electron microscopy. The magnetic properties of the compounds studied by SQUID magnetometry and element specific X-Ray magnetic circular dichroism (XMCD) confirm a robust ferrimagnetic order in agreement with the DFT calculations. The results provide a valuable framework for engineering new single-phase multiferroics with ferroelectrically active A -site cations.

- [1] Y. Krockenberger *et al.*, Phys. Rev. B **75**, 020404(R) (2007).

TT 77.6 Thu 16:30 H34

Structural and magnetic properties of orthorhombic ErFeO_3 from first principles — ●DOMINIK M. JURASCHEK and NICOLA A. SPALDIN — Materials Theory, ETH Zürich, Switzerland

We investigate the structural and magnetic properties of orthorhombic ErFeO_3 using density functional theory.

Rare-earth orthoferrites ($R\text{FeO}_3$) show complex coupled lattice and magnetic properties leading to interesting multiferroic, magnetoelectric and spin-dynamic behaviour.

We find that the PBEsol implementation of the generalized gradient approximation plus Hubbard U (GGA+U) method gives structural properties in good agreement with experiment. Using this approximation, we calculate the lattice dynamical properties, the magnetic ground state and the spin-phonon coupling. Our DFT calculations with erbium's 4f electrons frozen in the pseudopotential cores reproduce the G_x -type antiferromagnetic ordering with weak ferromagnetic

F_z canting that is observed experimentally at high temperatures. This lends support to the proposal that the observed spin reorientation transition at 100 K to a G_z ordering is mediated by coupling to erbium's 4f moments.

TT 77.7 Thu 16:45 H34

First-principles calculations on anion doped GaFeO₃ —
•JACQUELINE ATANELOV and PETER MOHN — Technische Universität Wien, Institut für Angewandte Physik, Computational Materials Science

We present ab initio DFT calculations performed on stoichiometric and anion doped GaFeO₃ substituting O by a C, N and S atom, respectively. Stoichiometric GaFeO₃ has an antiferromagnetic (AFM) ground state. The Fe atoms of the sublattices Fe1 and Fe2 couple antiferromagnetically via the O atoms through the superexchange mechanism. Exchanging the for the superexchange important O atom with p-elements of a different valence electron configuration changes the underlying magnetic exchange mechanism and influence the ground state properties which can be used for tuning properties interesting for technical applications. Four different doping configurations were examined revealing a cell site dependent influence on the magnetic properties. Carbon, for example, changes the AFM coupling present in the Fe1-O-Fe2 configuration into a ferrimagnetic exchange for the Fe1-C-Fe2 bond. Depending on the respective cell site C substitution introduces a ferrimagnetic or AFM ground state. Nitrogen alters the ground state magnetic moment as well and Sulfur introduces large structural distortions affecting the, band gap and the overall AFM coupling inside the doped GaFeO₃ simulation cell. We give a detailed discussion on the respective magnetic exchange mechanisms and electronic properties with regard to applications as photocatalysis and use the predictive power of ab initio DFT simulations that may trigger future experiments.

TT 77.8 Thu 17:00 H34

Multiferroicity in off-stoichiometric Ga_xFe_{1-x}O₃ —
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The recently reported observation of room-temperature multiferroic be-

havior in Ga_{0.6}Fe_{1.4}O₃ (GFO) [1] and ϵ -Fe₂O₃ (ϵ FO) [2] offers new perspectives for electronic devices whose operation is based on the switching of magnetic and electric ferroic ordering, as well as on the strong interaction between the magnetic and ferroelectric order parameters, such as multistate non-volatile memory cells. Unfortunately, the realistic microscopic switching mechanism is still not known for either of these materials. They are isostructural with polar Pna2₁ crystalline symmetry. In GFO, disorder in the occupancy of Ga and Fe sites is present, whereas ϵ FO is a fully ordered compound. Their parallel study allows us to understand the influence of disorder on possible ferroelectric properties, and develop criteria to maximize the effect. We will present the results of an evolutionary-algorithm [3] based study of GaFeO₃-Fe₂O₃ solid solutions, (i.e., with increasing iron content). We will show the condition at which the proper ferroelectricity arises in GFO multiferroics and characterize the parameters of the ferroelectric phase transition. – We acknowledge financial support by Helmholtz Young Investigators Group Programme VH-NG-409 and through DFG-ANR (GALIMEO Consortium).

[1] A. Thomasson *et al.*, J. Appl. Phys. **113**, 214101 (2013); [2] M. Gich *et al.*, Adv. Mater., **26**, 4645 (2014); [3] <http://uspex.stonybrook.edu>

TT 77.9 Thu 17:15 H34

Fine-tuning ferroic properties: an X-ray diffraction study of type-II multiferroics — •YOAV WILLIAM WINDSOR¹, MAHESH RAMAKRISHNAN¹, KENTA SHIMAMOTO², AURORA ALBERCA¹, LAURENZ RETTIG¹, ELISABETH MONICA BOTHSCHAFTER¹, YI HU², THOMAS LIPPERT², CHRISTOF SCHNEIDER², and URS STAUB¹ — ¹Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — ²General Energy Research Department, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

We present a complete X-ray diffraction study of high-quality crystalline films of a prototypical multiferroic, using soft and hard X-rays. With the prospect of future multiferroic functionalities in mind, we show that epitaxial strain directly controls both of the system's ferroic properties. We demonstrate that strain can be used to "push" the system between different multiferroic phases, and even to fine-tune the magnetic ordering periodicity. We generalize this to show that manipulating the crystal structure by other means allows fine-tuning the ferroic properties in a similar manner.