## DF 4: Multiferroics II (jointly with MA, DS, KR, TT)

Time: Monday 15:00–18:30 Location: EB 301

Invited Talk DF 4.1 Mon 15:00 EB 301

Anisotropic conductance of ferroelectric domain walls —

•Dennis Meier — Dept. of Physics, University of California, Berkeley, USA

Domain walls are natural interfaces that can exhibit structural, physical, and chemical properties which drastically differ from the surrounding bulk material. This applies to a large variety of phenomena including chemical/electrical transport, multiferroicity, or superconductivity. In addition to the fascinating physical properties domain walls are small in size and their position can be controlled rendering them interesting for future device design. In my talk I report on the exotic nature of trimerization-polarization domain walls in hexagonal ErMnO<sub>3</sub>. Using piezoforce-response microscopy and conductive atomic force microscopy we revealed that the domain walls represent a structural discontinuity being electrically dressed. While the structural component basically guarantees stability, the electrical dressing generates interesting and new nanoscale physics that I will discuss. The ferroelectric domain walls in ErMnO<sub>3</sub> for instance exhibit highly anisotropic electrical properties resulting in directional domain wall conductance. Remarkably, the local electrical conductance is a continuous function of the domain wall orientation which can be explained as a combined consequence of electrostatic and band-structure changes  $\,$ at the walls.

DF 4.2 Mon 15:30 EB 301

Structures and energetics of domain walls in polar hexagonal manganites — •Yu Kumagai and Nicola Spaldin — Department of Materials, ETH Zurich

We use first-principles density functional calculations to study the domain walls in the multiferroic hexagonal manganites, h- $RMnO_3$  (R=Sc, Y, Dy–Lu). These materials show an improper ferroelectricity induced by structural trimerization, resulting in  $2\times 3=6$  domains (2 for ferroelectricity and 3 for trimerization origin) below the Curie temperature with an intriguing cloverleaf pattern of domains [1,2]. Our calculations explain the observation that ferroelectric (FE) domain walls exist only in combination with antiphase DWs. We find that interlocked ferroelectric and antiphase domain walls have lower energies than typical FE domain walls in conventional ferroelectrics, as well as a much narrower wall width; both factors result from the layered geometry of the h- $RMnO_3$  structure.

- [1] T. Choi et al., Nature Mater. 9, 253 (2010).
- [2] T. Jungk et al., Appl. Phys. Lett. 97, 012904 (2010).

DF 4.3 Mon 15:45 EB 301

Hexagonal InMnO $_3$  - An Outsider Among The Family Of Multiferroic Hexagonal Manganites — •Martin Lilienblum $^1$ , Yu Kumagai $^1$ , Alexei A. Belik $^2$ , Naemi Leo $^1$ , Nicola A. Spaldin $^1$ , and Manfred Fiebig $^1$  —  $^1$ Department of Materials, ETH Zurich —  $^2$ International Center for Materials Nanoarchitectonics, NIMS

So far, it was believed that hexagonal (h-)  $InMnO_3$  exhibit the same type of multiferroic order as the other compounds from the h-RMnO<sub>3</sub> family (R = Sc, Y, Dy - Lu), including, in particular, a unit-cell-tripling improper ferroelectric order. Here we present experimental evidence for the absence of ferroelectricity in hexagonal InMnO<sub>3</sub> based on three different techniques: x-ray diffraction (XRD), piezoresponse force microscopy (PFM) and optical second harmonic generation (SHG). XRD data are ambiguous because they can be described likewise by the nonferroelectric  $P\bar{3}c$  structure and by the ferroelectric  $P6_3cm$  structure present in the other h-RMnO<sub>3</sub> compounds. However, PFM at room temperature and SHG measurements at low temperature uniquely reveal the absence of ferroelectric order in InMnO<sub>3</sub>. We therefore propose that InMnO<sub>3</sub> exhibits antiferrodistortive, but non-ferroelectric order according to the  $P\overline{3}c$  symmetry. Density functional calculations show that the relative energy between the  $P\overline{3}c$  and  $P6_3cm$  structures is determined by a competition between electrostatic and covalency effects, with an absence of covalency favoring the ferroelectric structure. We gratefully acknowledge the support by DFG through SFB 608.

DF 4.4 Mon 16:00 EB 301

Direct observation of multiferroicity in TbMnO<sub>3</sub> thinfilms
— ◆Artur Glavic<sup>1</sup>, Jörg Voigt<sup>1</sup>, Enrico Schierle<sup>2</sup>, Eugen

Weschke², and Thomas Brückel¹ — ¹Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszeutrum Jülich GmbH, Jülich, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Albert-Einsteinstr. 15, Berlin, Germany

Multiferroic rare earth manganites as  ${\rm TbMnO_3}$  have been studied a lot in the past ten years because of their complex magnetic structure, which leads to a ferroelectric polarization. So far investigations on  ${\rm TbMnO_3}$  thin films grown on LaAlO<sub>3</sub> or  ${\rm SrTiO_3}$  showed an emergent ferromagnetism, destroying the multiferroic properties.

We have investigated  $TbMnO_3$  films grown with sputter deposition on YAlO $_3$  substrates using soft x-ray resonant magnetic scattering with linear and circular polarized light. By measuring the circular dichroism originating from the chirality of the magnetic structure we could directly observe multiferroic domains in the thin films. Although the transition temperatures found were comparable to bulk, an additional influence of the Tb magnetic order on the ferroelectricity was observed.

DF 4.5 Mon 16:15 EB 301

Sinusoidal electromagnon in RMnO<sub>3</sub>: Indication of anomalous magnetoelectric coupling — •MARKKU STENBERG¹ and Rogério de Sousa² — ¹Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — ²Department of Physics and Astronomy, University of Victoria, Victoria, B.C., V8W 3P6, Canada

The optical spectra in the family of multiferroic manganites  $RMnO_3$  is a great puzzle. Current models can not explain the fact that two strong electromagnons are present in the non-collinear spin cycloidal phase, with only one electromagnon surviving the transition into the collinear spin sinusoidal phase. We show that this is a signature of the presence of anomalous magnetoelectric coupling that breaks rotational invariance in spin space and generates oscillatory polarization in the ground state.

DF 4.6 Mon 16:30 EB 301

Neutron scattering studies on chiral multiferroics: magnetic structure and excitations —  $\bullet \text{Max}$  Baum¹, Thomas Finger¹, Jeannis Leist², Karin Schmalzl³, Paul Steffens³, Petra Becker⁴, Ladislav Bohaty⁴, Götz Eckold², and Markus Braden¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Institut für Physikalische Chemie, Georg-August-Universität Göttingen — ³Institut Laue Langevin (ILL), Grenoble — ⁴Institut für Kristallographie, Universität zu Köln

Multiferroic materials or compounds with a strong magnetoelectric effect posses a large application potential in data storage techniques. Quite recently, systems with a peculiar spiral magnetic order were shown to directly induce a spontaneous electric polarisation and to exhibit giant magnetoelectric effect. Neutron scattering with spherical polarisation analysis gives access to the chiral component of the magnetic structure which is directly linked to the electric polarisation. Therefore, it is possible to control the chiral components by an external electric field. We present neutron scattering experiments on IN14 and IN20 using spherical polarisation analysis documenting the poling of the elastic magnetic chiral terms for MnWO4, TbMnO3 and Ni3V2O8 by cooling in an electric field. In addition, it is possible to switch the chiral components by varying the electric field at constant temperature; thereby measuring multiferroic hysteresis curves. For MnWO4, this experiment was performed with time resolution detecting the typical relaxation times. Tor TbMnO3 we discuss a newly discovered excitation which exhibits a chirality opposite to the static one.

DF 4.7 Mon 16:45 EB 301

Theoretical study of Magnetoelectric effects in Multiferroic RMn2O5 —  $\bullet {\rm Safa}$  Golrokh Bahoosh¹, Julia Wesselinowa², and Steffen Trimper³ —  $^1{\rm Max}$  Planck Institute of Microstructure Physics, 06099 Halle, Germany —  $^2{\rm Department}$  of Physics, University of Sofia, 1164 Sofia, Bulgaria —  $^3{\rm Institute}$  of Physics, Martin-Luther-University, 06120 Halle, Germany

The magnetoelectric behavior of the rare-earth RMn2O5 perovskites is studied theoretically using a quantum model. Whereas the magnetic subsystem is described by nearest-neighbor ferromagnetic coupling and next nearest neighbor antiferromagnetic order, the ferroelectric subsystem is characterized by an Ising model in a transverse field.

Due to frustration, the magnetic system offers spiral structures. The coupling between both systems is a symmetry-allowed linear coupling.

Using Green\*s functions we find analytically the temperature and wave vector dependent elementary excitation of the Magnetoelectric system, the polarization and the magnetization for different magnetoelectric coupling strengths.

Lowering the temperature, the system undergoes a magnetic transition at TN and a further reduction of the temperature leads to a ferroelectric transition at TC < TN. The magnetoelectric coupling is manifested as a kink in both the magnetization and the elementary excitation at TC. The polarization is enhanced under the presence of a finite external magnetic field. In the same manner the magnetization is slightly changed by an applied electric field near to TC.

## 15 min. break

DF 4.8 Mon 17:15 EB 301

Origin of spin canting in multiferroic perovskites — •Carlo Weingart, Eric Bousquet, and Nicola Spaldin — Materials Department, ETH Zurich, Switzerland

In magnetic perovskites with oxygen octahedral distortions, it is usually admitted that the Dzyaloshinsky-Moriya interaction (DM) is responsible for the spin canting. This statement is however partially true since the single-ion anisotropy (SIA) can also allow for similar spin canting. By decomposing the different magnetic interactions (exchange, DM and SIA) from first-principles calculations, we show that depending on the magnetic cation, the DM and the SIA can be of similar amplitude. This allow us to reconsider the origin of the weak ferromagnetism in multiferroics.

DF 4.9 Mon 17:30 EB 301

A further step of understanding the complex magnetic order in magnetoelectric Co<sub>3</sub>TeO<sub>6</sub> — •Vera Carolus<sup>1</sup>, Thomas Lottermoser<sup>2</sup>, Matthias Hudl<sup>3</sup>, Pierre Tolédano<sup>4</sup>, and Manfred Fiebig<sup>2</sup> — ¹HISKP, University of Bonn, Germany — ²Department of materials, ETH Zurich, Switzerland — ³Department of Engineering Sciences, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden — ⁴Laboratory of Physics of Complex Systems, University of Picardie, 33 rue Saint-Leu, 80000 Amiens, France

Like most of the known magnetoelectric multiferroics,  $\mathrm{Co_3TeO_6}$  exhibits a complex spin structure with a series of consecutive phase transitions. Contrary to common compounds,  $\mathrm{Co_3TeO_6}$  possesses two independent commensurate k-vectors in the multiferroic low-temperature phase. In addition, magnetic-field dependent measurements of the ferroelectric polarization show a strongly anisotropic behaviour.

Here we show our results using spatially resolved optical second harmonic generation (SHG) under external magnetic and electric fields in the multiferroic low-temperature phase. However, the SHG gives only access to the magnetic subsystem. Like the ferroelectric polarization, the magnetic structure shows strongly anisotropic behaviour. In crossed magnetic and electric fields we were able to reach a single-domain state, while a magnetic field solely always leads to distinctively different multi-domain states. Most remarkably, for a certain direction of magnetic field, we were able to invert the multi-domain state. Furthermore, this behaviour indicates the existence of a pronounced memory effect.

DF 4.10 Mon 17:45 EB 301

The multiferroic, geometric frustrated CuCrO $_2$  compound: a case of the p-d hybridization spin-charge coupling? — •MATTHIAS FRONTZEK, GEORG EHLERS, and ANDREY PODLESNYAK — Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Multiferroic materials have become of interest for their unusual low-

temperature properties in general, and in particular for the observation that one can affect their magnetic structure through an electric field and their electric polarization through a magnetic field. The delafossite CuCrO<sub>2</sub>, which crystallizes in the rhombohedral  $R\overline{3}m$  space group, is a multiferroic compound with an apparent strong coupling of spin and charge. In contrast to other multiferroic compounds CuCrO<sub>2</sub> shows a spontaneous electric polarization upon antiferromagnetic ordering without an accompanying structural phase transition, although a slight in-plane lattice distortion has been measured.

In our contribution, we present a detailed study on CuCrO<sub>2</sub> single crystals using neutron diffraction and spectroscopy as well as pulsed magnetic field measurements up to 60 T of the electric polarization. Based on our study we will show a revised magnetic structure model and present a model Hamiltonian including in-plane next-next nearest neighbor and inter-layer exchange interaction. We will stress the importance of the latter for the multiferroic properties and will show evidence based on the high field polarization measurements that the proposed p-d hybridization spin-charge coupling mechanism needs to be modified.

DF 4.11 Mon 18:00 EB 301

Theory of High-Temperature Multiferroicity in CuO — •Naëmi Leo<sup>1,2</sup>, Pierre Tolédano<sup>3</sup>, Dmitry D. Khalyavin<sup>4</sup>, and Manfred Fiebig<sup>1,2</sup> — <sup>1</sup>ETH Zurich, Switzerland — <sup>2</sup>HISKP, Universität Bonn, Germany — <sup>3</sup>University of Picardie, France — <sup>4</sup>ISIS, United Kingdom

Spin-spiral multiferroics offer strong magnetoelectric coupling, although most of them have low transition temperatures which make them undesirable for technical applications. Cupric oxide is a remarkable exception with its high Curie temperature of 230 K. Understanding the interactions leading to such a high- $T_C$  magnetically induced ferroelectricity is very desirable for future room-temperature magnetoelectric multiferroics devices.

Here we present a Landau theory analysis of the multiferroic properties of CuO [1]. Using a multi-dimensional order parameter expansion of the free energy we examine the sequence of phase transitions: The unusual direct transition to the multiferroic phase is induced by the simultaneous onset of two order parameters, enabled by the strong Cu-O superexchange. Expressing the order parameter in terms of spins we determine theoretically the magnetic structure in the spin-spiral phases. Furthermore we identify the microscopic interactions responsible for the magnetically induced spontaneous polarization.

The work in Bonn was supported by the DFG through the SFB 608. [1] P. Toledano, N. Leo, D.D. Khalyavin, L.C. Chapon, T. Hoffmann, D. Meier, and M. Fiebig, Phys. Rev. Lett. **106**, 257601 (2011).

DF 4.12 Mon 18:15 EB 301

Resonant Elastic X-ray Scattering Studies of Multiferroic  $NdFe_3(BO_3)_4$  — •Sven Partzsch<sup>1</sup>, Jorge Enrique Hamann-Borrero<sup>1</sup>, Claudio Mazzoli<sup>2</sup>, A. Vasiliev<sup>3</sup>, L. Bezmaternikh<sup>4</sup>, Bernd Büchner<sup>1</sup>, and Jochen Geck<sup>1</sup> — <sup>1</sup>IFW, Dresden, Germany — <sup>2</sup>ESRF, Grenoble, France — <sup>3</sup>Moscow State University, Moscow, Russia — <sup>4</sup>L. V. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia

Multiferroic NdFe<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> exhibits a strong magnetoelectric coupling, since at 2K the electric polarization raises rapidly to  $400\,\mu\text{C/m}^2$  upon increasing the applied magnetic field to 2T [1]. We study this coupling by resonant x-ray scattering at the Nd L- and Fe K edges as a function of temperature and applied magnetic field. Employing full polarization control, the field dependence of the different magnetic phases has been characterized at the Nd  $L_2$  edge. We find that the commensurate phase at 20K and no magnetic field is different from the commensurate phase induced by the magnetic field at 2K [2].

[1] A. Zvezdin et al., JMMM, 300, 224 (2006)

[2] J. E. Hamann-Borrero et al., Phys. Rev. B, 82, 094411 (2010)