TT 2: Multiferroics 1 (jointly with DF, DS, KR, and MA)

Time: Monday 9:30–12:00 Location: H3

TT 2.1 Mon 9:30 H3

Magnetoelectric coupling at the n-doped interface $BaTiO_3/SrTcO_3$ studied from first principles — •Vladislav Borisov[1], Sergey Ostanin[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Antiferromagnetically induced magnetoelectric coupling at the interface $BaTiO_3/SrTcO_3$, which combines a robust ferroelectric and a stable antiferromagnetic perovskite, is studied from first principles. For the BaO/TcO_2-terminated interface, the magnetic order may change from G- to C-type antiferromagnetism upon the electric polarization reversal in the ferroelectric side. By inspecting the two-dimensional band structure and orbital occupation of the Tc 4d-states we conclude that the polarization-dependent charge transfer is responsible for a two-dimensional electron gas at the interface between two insulating perovskites. The case of paraelectric $BaTiO_3$ is also discussed in the context of the effect.

TT 2.2 Mon 9:45 H3

Observation of novel multiferroic-like effect in C60-Co nanocomposites — •Masashi Shiraishi[1], Eiiti Tamura[1], Yutaka Sakai[1], Toyokawa Shuhei[1], Eiji Shikoh[1], Vlado Lazarov[2], Atsufumi Hirohata[3], Teruya Shinjo[1], and Yoshishige Suzuki[1] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]Department of Physics, Univ. York, UK — [3]Department of Electronics, Univ. York, UK

A novel magnetoelectric effect is found to appear in a C60-Co nanocomposite. Although Co is well-known as a ferromagnet, its nanoparticles embedded in a C60 matrix can exhibit enhancement of magnetoresistance ratio due to a combination of Coulomb-blockade and higher order co-tunneling [1], and also multiferroic-like behavior [2], i.e., an electric field controls magnetic alignment of the nanoparticles and a magnetic field controls their charged states. This novel effect enables a strong magnetic switching effect for which the on/off ratio is ca. 1e4. Such an effect has been expected to exist and these findings show this magnetoelectric coupling for the first time.

[1] D. Hanataka, M. Shiraishi et al., Phys. Rev. B79, 235402 (2009).
[2] Y. Sakai, E. Tamura, M. Shiraishi et al., Adv. Func. Mat. 22, 3845 (2012).

TT 2.3 Mon 10:00 H3

Investigation of magnetic ordering in $Eu_{1-x}Y_xMnO_3$ using full polarization analysis at P09 beamline — •Arvid Skaugen, Dinesh K. Shukla, Helen Walker, Sonia Francoual, and Jörg Strempfer — Deutsches Elektronen-Synchrotron, Harmburg, Germany

Varying multiferroic properties with strong ME coupling have been reported for $Eu_{1-x}Y_xMnO_3$ [1]. The crystal structure of $Eu_{1-x}Y_xMnO_3$ is similar to the one of $TbMnO_3$ with comparable lattice distortions. However, the effect of rare earth magnetism is eliminated since Eu^{3+} ($4f^6$) and Y^{3+} ($4f^0$) ions both are non-magnetic. The compound $Eu_{0.8}Y_{0.2}MnO_3$ first shows a phase transition at T_N = 45K from a paramagnetic to an antiferromagnetic and paraelectric state with a presumably sinusoidal collinear AFM structure, in analogy to $TbMnO_3$. At T_C = 30K the magnetic structure changes to weak ferromagnetism, attributed to a cone-like structure that breaks inversion symmetry and gives rise to ferroelectricity with the polarization along the a-axis.

We have investigated $Eu_{0.8}Y_{0.2}MnO_3$ using resonant x-ray diffraction as function of temperature, magnetic field and incident polarization at beamline P09 at PETRA III. The method of full polarization analysis has been used to investigate the different resonances showing up at the Mn K-edge. From the polarization scans, it is possible to draw conclusions on the complex magnetic order. Preliminary results suggest a helicoidal SDW structure of the Mn moments rather than a cone-like structure.

[1] J. Hemberger et al., Phys. Rev. B 75, 035118 (2007)

TT 2.4 Mon 10:15 H3

Electrostatic tuning of large-distance sputtered LSMO/PZT heterostructures — •Philipp Moritz Leufke, Ajay Kumar Mishra, Wang Di, Robert Kruk, and Horst Hahn — Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

In order to obtain a physical picture and quantitative characteristics of a magnetoelectric coupling at ferromagnetic/ferroelectric interfaces, epitaxial $La_{0.87}Sr_{0.13}MnO_3/Pb(Zr,Ti)O_3$ (LSMO/PZT) heterostructures were deposited by large-distance magnetron sputtering[1,2]. The remarkably high lateral uniformity achieved in such films allowed for a ferroelectric device area of more than 6 mm^2.

This has enabled for the first time *in-situ* SQUID measurements of the magnetic response to the systematically varied remanent ferroelectric polarization. Temperature dependence of the magnetic modulation upon charging and the magnetic response to the ferroelectric stimulation indicates a field-effect dominated coupling mechanism and generally confirms the concept of electrostatic hole (h^+) doping of LSMO.

For small charge modulations at low temperature, a linear tuning coefficient of $\approx 3.6\,\mu_B/h^+$ has been determined. This suggests the activation of an antiferromagnetic coupling, even for very small surface charge densities. Simultaneously a shift in the magnetic transition temperature at higher surface charge concentration indicates the presence of a ferromagnetic phase at the LSMO/PZT interface.

[1] P. M. Leufke *et al.*, *Thin Solid Films* **520**, 5521 (2012).
[2] P. M. Leufke *et al.*, *AIP Advances* **2**, 032184 (2012).

TT 2.5 Mon 10:30 H3

Optimized magnetoelectric interface coupling — •Igor Maznichenko[1], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany

It was shown that magnetoelectric coupling occurs at interfaces between a magnetic and a ferroelectric material. Our idea is to construct heterostructures with a particularly strong magnetoelectric coupling. We concentrate on the optimization of the magnetic layer. We demonstrate that a small magnetic moment at the interface can still transfer the magnetoelectric coupling to a strong ferromagnet and could cause significant response. The idea is supported by numerical simulations within density functional theory using the self-consistent KKR Green function method.

TT 2.6 Mon 10:45 H3

Role of electron correlation of FeO at Fe/ferroelectric oxide/Fe interface for magnetic transport properties — •Andrea Neroni, Daniel Wortmann, Ersoy Sasioglu, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Fe/ferroelectric oxide/Fe is a nanoferronic tunnel junction with exciting electronic magneto-conductive transport properties. FeO layers at the interface of Fe/oxide/Fe barriers seems to significantly alter these properties as indicated by several experiments. In order to understand the role of electron correlations in FeO at the interface on the tunneling properties of a $Fe/BaTiO_3/Fe$ barrier we use an embedded Green-function approach [1] implemented within the framework of the full-potential linearized augmented plane-wave (FLAPW) method `FLEUR` [2]. Conductances are obtained for different oxidation conditions and for different magnetic configurations of the contacts. Strong correlations are taken into account employing the LDA+U approach within the framework of the density functional theory (DFT) with a Hubbard U parameter determined by constrained random phase approximation (cRPA) [3]. Work is supported by Helmholtz Young Investigators Group Program VH-NG-409.

[1] www.flapw.de
[2] D. Wortmann, H. Ishida, and S. Blügel, PRB **65**, 165103 (2002)
[3] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011)

TT 2.7 Mon 11:00 H3

Multiferroic Aurivillius Phases: the Case of $Bi_5FeTi_3O_{15}$ by *ab initio* — •Yael Birenbaum, Nicola Spaldin, and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

The Aurivillius phases form a family of naturally-layered perovskite-

related materials with good ferroelectric properties. $Bi_5FeTi_3O_{15}$ (BFTO) is perhaps the simplest known member of this family that also incorporates magnetic degrees of freedom. Using *ab initio* electronic structure calculations, we establish the ferroelectric and magnetic properties of BFTO. We then discuss a possible site preference of the Fe^{3+} cation, which so far has not been found experimentally, and quantify the magnetic coupling between adjacent Fe cations. In addition, we analyse the different structural distortions, in order to relate BFTO to other members of the Aurivillius phases.

TT 2.8 Mon 11:15 H3

Strain effect on magnetic properties of $La_{0.7}Ca_{0.3}MnO_3/SrRuO_3$ Superlattices — •Sujit Das[1,2], Andreas Herklotz[1,2], and Kathrin Doerr[1,2] — [1]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [2]Institute for Physics, MLU Halle-Wittenberg, 06099 Halle, Germany

Coherent interfaces between magnetic oxides such as $La_{0.7}$ $Sr_{0.3}MnO_3$ and $SrRuO_3$ may induce an intense magnetic coupling [1]. Recent work indicated an impact of elastic strain on the strength and even the sign of the coupling [2]. Superlattices (SL) of $La_{0.7}$ $Ca_{0.3}MnO_3/SrRuO_3$ with layer thicknesses below 10 unit cells were grown by pulse laser deposition simultaneously on $SrTiO_3$(001) (STO), $LaAlO_3$(001) (LAO) and piezoelectric $0.72Pb(Mg_{1/3}Nb_{2/3})O_3$-$0.28PbTiO_3$ (001) (PMN-PT) substrates and structurally characterized by X-ray diffraction (XRD). On LAO, the SL assumes a compressive strain state, i. e. the lattice parameter is larger out-of-plane than in-plane, whereas on PMN-PT it shows a tensile strain state and on STO an intermediate strain value. Magnetization measurements demonstrate a strong antiferromagnetic (AFM) coupling in SLs on STO and LAO substrates which is due to superexchange interaction between Ru and Mn ions. The AFM coupling seems to decrease under tensile strain. The coupling is much weaker on PMN-PT, probably because of higher interface roughness. In order to probe the effect of elastic strain directly, magnetization loops in reversibly controlled strain states have been recorded for SLs on PMN-PT. [1] M. Ziese et al., PRL 104, 167203 (2010), [2] J. W. Seo et al., PRL 105, 167206 (2010) .

TT 2.9 Mon 11:30 H3

Tuning the multiferroic phase of CuO with impurities — •Johan Hellsvik[1], Marcello Balestieri[1], Alessandro Stroppa[2], Anders Bergman[3], Lars Bergqvist[4], Olle Eriksson[3], Silvia Picozzi[2], and José Lorenzana[1] — [1]ISC-CNR, Rome, Italy — [2]CNR-SPIN, L'Aquila, Italy — [3]Uppsala University, Uppsala, Sweden — [4]KTH, Stockholm, Sweden

The discovery that CuO is a multiferroic with a high antiferromagnetic transition temperature of 230 K opened a possible route to room-temperature multiferroicity with a strong magnetoelectric coupling [1]. CuO belongs [2] to a new class of multiferroic materials where the so called 'order by disorder mechanism' [3] plays a crucial role. In this work we study the effect of different impurities on the phase diagram of CuO aiming at engineering the multiferroic properties. Extensive density functional theory (DFT) calculations were performed for a large number of fixed spin configurations in pure CuO and CuO doped with a small fraction of the Cu atoms substituted with the nonmagnetic elements Mg, Zn or Cd, or the magnetic elements Ni or Co. Our computations established that the energy difference between the low-temperature collinear AF1 phase and the intermediate temperature multiferroic AF2 phase decreased monotonously with increasing doping level confirming that impurities favour the multiferroic phase. The magnetic phase diagram has been mapped out in Monte Carlo simulations for classical Heisenberg spins. [1] T. Kimura et al., Nature Mat. 7, 291 (2008); [2] G. Giovannetti et al., Phys. Rev. Lett. 106, 026401 (2011); [3] C. L. Henley, Phys. Rev. Lett. 62, 2056 (1989)

TT 2.10 Mon 11:45 H3

Charge-mediated magnetoelectric coupling in patterned multiferroic heterostructures — •daniele preziosi[1], dietrich hesse[1], marin alexe[1], martin wahler[2], and georg schmidt[2] — [1]Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, 06120 Halle(Saale) Germany — [2]Martin-Luther-Universität Halle-Wittenberg Von-Danckelman-Platz 3, 06120 Halle(Saale) Germany

Several studies on single phase multiferroics demonstrate that the coupling between the ferroelectric and the (ferro)magnetic order parameters tends to be small. Engineering of artificially structured systems could provide a reliable way to improve the MagnetoElectric (ME) coupling. Devices based on charge-mediated ME effect represent a viable alternative. The electric field produced by the polarization of the ferroelectric material can induce, at the interface with an ultrathin strongly correlated magnetic oxide, a change in the magnetization. The ME coupling would be in this case the consequence of the spin-dependent screening of the electric field. Patterned hetero-structures of La1-xSrxMnO3 (LSMO) and PbZr0.2Ti0.8O3 (PZT) have been fabricated. Transport and magnetic measurements show that the switching of the PZT polarization influences significantly the competing electronic ground states of the LSMO, modulating the resistivity as well as the magnetization value.