# DF 2: Multiferroics I (jointly with MA, DS, KR, TT)

Time: Monday 9:30–12:45 Location: EB 301

**Topical Talk** DF 2.1 Mon 9:30 EB 301

**Reversible electrical switching of spin polarization in multiferroic tunnel junctions** — •Marin Alexe, Daniel Pantel, Silvana Götze, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

Spin polarized transport in ferromagnetic tunnel junctions, characterized by tunnel magnetoresistance, has already proven a high application potential in the field of spintronics and in magnetic random access memories (MRAM). Until recently, in such a junction the insulating barrier played only a passive role keeping apart the ferromagnetic electrodes in order to allow electron tunneling. However, a new dimension was added to these devices by replacing the insulator with a ferroelectric material, which possesses permanent dielectric polarization switchable between two stable states. The obtained multiferroic tunnel junction (MFTJ) is a non-volatile memory device with four states, given by two possible ferroelectric polarization directions in the barrier and two different magnetization alignments of the electrodes. Here, we will show that due to the coupling between magnetization and ferroelectric polarization at the interface between a magnetic electrode and the ferroelectric barrier of a MFTJ, the spin polarization of the tunneling electrons can be reversibly and remanently inverted by switching the ferroelectric polarization of the barrier. Selecting the spin direction of the tunneling electrons by short electric pulses in the nanosecond range rather than by an applied magnetic field is highly relevant for spintronics, especially for spin-based information technology.

DF 2.2 Mon 10:00 EB 301

**First Principles Modelling of Spin Transport in Functional Oxide Tunnel Junctions** — •Nuala M. Caffrey, Thomas Archer, Ivan Rungger, and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Ireland

Spin-dependent tunnelling between ferromagnetic electrodes separated by insulating oxide barriers has long attracted scientific and commercial interest. In the last decade it became evident that the insulating layer was more than just a simple barrier through which electrons tunnel. It is wave-function symmetry selective, making the tunnelling process sensitive to its electronic structure. The understanding of such a concept suggests that one can engineer the transport properties of a tunnel junction by carefully selecting the insulating barrier and the metallic electrodes. Ferroelectric materials are of particular interest as barriers due to additional functionality offered by the electric polarisation.

We investigate, from first-principles, the properties of a multifunctional tunnel junction combining two materials with different ferroic states (ferromagnetic and ferroelectric). We demonstrate massive tunnelling magnetoresistance (TMR) in a SrRuO3 / BaTiO3 / SrRuO3 junction. We also consider the implications of introducing structural asymmetry into this junction by using a thin layer of dielectric material at one interface. In such a junction we demonstrate a sizable tunnelling electroresistance (TER) that increases with the thickness of the dielectric layer.

DF 2.3 Mon 10:15 EB 301

**FeO at Iron/Oxide interfaces** — •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

We present density-functional theory (DFT) based first-principles calculations of tunneling and magnetoconductance properties of nanoferronic devices consisting of oxide barriers between iron contacts. Several experimental works have indicated the presence of an iron-oxide layer at the contacts of this barrier, that can significantly alter the tunneling properties of the junction. The effect of this layer is still unclear. From the theoretical point of view, one unexplored point are the electron correlations in the single FeO layer at the interface. We account for these correlations with a Hubbard U parameter determined by the constrained random phase approximation (cRPA) [1] and calculate the change of the tunneling magnetoresistance ratio under this condition, using the full-potential linearized augmented plane wave (FLAPW) method `FLEUR` [2]. The electronic transport properties of nanoferronic junctions have been investigated using an embedded Green-function approach [3].

Work is supported by Helmholtz Young Investigators Group Program VH-NG-409 .

[1] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011)
[2] www.flapw.de
[3] D. Wortmann, H. Ishida, and S. Blügel. PRB **66**, 075113 (2002)

DF 2.4 Mon 10:30 EB 301

**Thermally stimulated currents in $BiFeO_3$** — •Akash Bhatnagar, Ayan Roy Chaudhuri, Dietrich Hesse, and Marin Alexe — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle(Saale), Germany

Bismuth ferrite($BiFeO_3$)-BFO is a well known multiferroic material, with high ferroelectric Curie temperature (1103 K) and a saturated ferroelectric hysteresis with a remnant polarization of 100 $C/cm^2$. However, it has been found that pure BFO usually exhibits a high leakage current that could limit wide applications of this material. The thermally stimulated current (TSC) technique was used to get insights into the electronic origin of the leakage, which includes the study of energy levels that might be present in the band gap. These levels can act as trapping centers for charge carriers, thus affecting conductivity. Three systems of BFO, namely, single crystals, thin films and ceramics were studied. Measurements for ceramics and single crystals were performed in capacitor mode, whereas for thin films in-plane electrodes were made using a normal lift-off process. The effect of orientation of the electrodes with respect to domain patterns in thin films, have been investigated. Consequently, trap activation energies and density calculations were performed to fully characterize different levels. Photoconductive and photovoltaic properties were also investigated which corroborate the TSC data.

DF 2.5 Mon 10:45 EB 301

**Preparation and characterization of multiferroic thin films grown with an Oxid-MBE** — •Paul Zakalek, Markus Waschk, Alexander Weber, and Thomas Brückel — Jülich Centre for Neutron Science JCNS und Peter Grünberg Institut PGI, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

An oxygen-assisted Molecular Beam Epitaxy (MBE) gives the possibility to engine artificial materials on a nanoscale with promising effects. With our machine it is possible to grow complex materials like $La_xSr_{1-x}MnO_3$ (LSMO) or $La_xBi_{1-x}MnO_3$ (LBMO) with remarkably good crystalline quality.

The materials show a variety of interesting effects. For example the La concentration affects the magnetic and electric properties of this systems. The LSMO and LBMO layers can either be antiferromagnetic, ferromagnetic or multiferroic, depending of the La concentration.

Different LSMO/LBMO systems were grown with oxygen-assisted MBE on a $SrTiO_3$ (STO) substrate with different La concentrations. We will present the preparation process and the structural in-house characterization of this systems. First results show good structural quality, like surface roughnesses of not more then one unit cell. Additionally magnetic and electric measurements of the samples will be shown.

**15 min. break**

DF 2.6 Mon 11:15 EB 301

**Guest molecules in ABX3 metal-organic frameworks: multiferroicity and magnetoelectricity** — •Alessandro Stroppa[1], Prashant Jain[2], Paolo Barone[1], Martijn Marsman[3], Juan Manuel Perez-Mato[4], Anthony K. Cheetham[5], Harold W. Kroto[2], and Silvia Picozzi[1] — [1]CNR-SPIN, L'Aquila, Italy — [2]Department of Chemistry and Biochemistry, Florida State University Tallahassee, FL 32306 (USA) — [3]University of Vienna, Faculty of Physics and Center for Computational Materials Science (Austria) — [4]Departamento de Fisica de la Materia Condensada Facultad de Ciencia y Tecnologia, UPV/EHU, Bilbao (Spain) — [5]Department of Materials Science and Metallurgy University of Cambridge (UK)

Metal-organic frameworks (MOFs) are increasingly regarded as promising materials. MOFs with perovskite architecture have recently branched out into the field of multiferroics, materials which have both magnetic and ferroelectric orders. Here, we focus on a MOF compound

and theoretically show that it is ferroelectric and this ferroelectricity is the cause of a weak ferromagnetic coupling. In inorganic perovskite-like compounds, octahedral tilting and Jahn-Teller distortions are usually non-polar modes. In this MOF, however, their cooperative link to A-groups via hydrogen bondings finally breaks inversion symmetry, and induces a ferroelectric polarization. We show that the switching of polarization direction implies the reversal of the weak ferromagnetic component, therefore allowing the long-sought electrical control of the magnetization.

DF 2.7 Mon 11:30 EB 301

**magnetoelectric effects in the cubic ferrimagnet $Cu_2OSeO_3$** — •Maria Eleni Belesi[1,2], Mohamed Abid[1], Helmuth Berger[1], and Jean-Philippe Ansermet[1] — [1]Institute of Condensed Matter Physics, EPFL, Station 3, CH-1015 Lausanne, Switzerland — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

We present magnetic and dielectric measurements in single crystals of the cubic magnetoelectric compound $Cu_2OSeO_3$. The magnetic measurements show a transition to a ferrimagnetic state at 60 K. This state shows a finite magnetocapacitance which is temperature dependent and varies significantly upon changing the direction of the magnetic field with respect to the crystallographic axes. The magnetocapacitance is also shown to vary with the relative orientation of the magnetic and electric fields. In addition, we found that the magnetically ordered state shows a magnetic field induced electric polarization, whose temperature dependence and anisotropic properties will be discussed.

DF 2.8 Mon 11:45 EB 301

**Microscopic Mechanisms for Magnetoelectric Effect in $LiMPO_4$ (M=Mn,Fe,Co,Ni)** — •Andrea Scaramucci, Eric Bousquet, and Nicola Spaldin — Materials Theory, Department of Materials, ETH Zurich, Zurich, Switzerland

We theoretically investigate the microscopic mechanisms leading to the linear magnetoelectric effect in the $LiMPO_4$ series. This is of particular interest since some of its constituents possess toroidal moments and shows large magnetoelectric effect.

By using symmetry analysis we obtain the microscopic couplings between spins and electric polarization responsible for each component of the magnetoelectric tensor. Furthermore, we identify couplings with exchange-strictive and relativistic origin. By using *ab initio* calculation and by enforcing numerous non collinear spin configurations we extract the strength of these couplings together with the exchange coupling constants. We use mean field approximation and Monte Carlo simulation to calculate the temperature evolution of magnetoelectric tensor. Our calculations explain the features of the temperature dependence found in experiments.

DF 2.9 Mon 12:00 EB 301

**Manipulation of the antiferromagnetic structure in $LiNi_{(1-x)}Fe_xPO_4$ (x = 0.03, 0.2) by iron substitution** — •Anne Zimmermann[1] and Manfred Fiebig[1,2] — [1]HISKP, University of Bonn, Germany — [2]Materials Department, ETH Zurich, Switzerland

The Li$M$PO$_4$ system ($M$ = 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 order to investigate the interplay between the different types of spin order $LiNi_{(1-x)}Fe_xPO_4$ samples with different mixing ratios of nickel and iron were studied using optical second harmonic generation (SHG). SHG coupling linearly to the AFM order parameter was identified in spectroscopy measurements and used for domain imaging. A small iron substitution of $x = 0.03$ yields no change in the domain pattern as well as in the magnetic structure in contrast to pure $LiNiPO_4$. However, for an iron substitution of $x = 0.2$ the spin structure changes significantly: the spin direction lies in the yz-plane and thus between the two spin directions for $LiNiPO_4$ and $LiFePO_4$. The change in magnetic structure is revealed in a different domain pattern as well. Furthermore the order parameter exhibits an unusual, photosensitive temperature dependence which is discussed in detail.

- Work supported by the SFB 608 of the DFG.

DF 2.10 Mon 12:15 EB 301

**Multiferroicity and magnetoelectricity in a doped topological ferroelectric** — Marco Scarrozza, Maria Barbara Maccioni, Giorgia M. Lopez, Alessio Filippetti, and •Vincenzo Fiorentini — Dept of Physics, U of Cagliari and CNR-IOM, Cagliari, Italy

$La_2Ti_2O_7$ is a "topological" ferroelectric where dipoles are produced by antiferrodistortive rotations failing to compensate due to the layered structure. To turn on multiferroicity, we investigated magnetic doping from first-principles within density-functional theory. The isovalent substitution of Mn for Ti produces antiferromagnetism at all dopings as expected due to superexchange between Mn $d^3$ ions. In the fully-substituted compound $La_2Mn_2O_7$, many ordering patterns compete, the lowest being a variant of G-type antiferromagnetism. The same system is also magnetoelectric, because the rotations are involved in both magnetic and ferroelectric order: as a coercive field undoes the rotations and depolarizes ferroelectricity, magnetic coupling doubles in intensity. However, the ferromagnetic phase of $La_2Mn_2O_7$ is always much higher in energy. On the other hand, we find that heterovalent substitution of Ti with Cr, Sc, and V always yields robust ferromagnetism. In particular, V orders in rows orthogonal to the P direction, with a covalency gap of 0.2 eV: $La_2Ti_{2-x}V_xO_7$ is therefore properly multiferroic. We are currently investigating the magnetoelectric tensors.

DF 2.11 Mon 12:30 EB 301

***Ab initio* study of the properties of $BaTiO_3$/Co-Pt alloy interface** — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA,52425 Jülich, Germany

Multiferroics are materials which exhibit more that one ferroic order parameter. They can be made of a single phase, where multiple ferroic order parameters co-exist simultaneously, or of composites, where different ferroic order parameters are combined in separate phases. Due to the limited number of known single phase multiferroics, most of which present multiple ordering only at low temperatures, engineering of composite junctions based on interfaces of magnetic and ferroelectric compounds are therefore of great scientific interest but are also promising due to their potential applications.

Cobalt-platinum alloys are known as compounds with a strong potential for applications in magnetic data storage, due to the strong exchange interactions and strong spin-orbit coupling (and, as a consequence, a large magnetocrystalline anisotropy energy). We present results of *ab initio* calculations based on density functional theory (DFT) of the magneto-electric coupling in cobalt-platinum alloys interfaced with $BaTiO_3$ ferroelectric.

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