Symposium Ferroic materials and novel functionalities (SYNF)

jointly organized by
Magnetism Division (MA),
Surface Science Division (O),
Metal and Material Physics Division (MM),
Dielectric Solids Division (DF),
Thin Films Division (DS),
Semiconductor Physics Division (HL), and
Low Temperature Physics Division (TT)

Ingrid Mertig
Fachgruppe Theoretische Physik
Fachbereich Physik
Universität Halle-Wittenberg
Von-Seckendorff-Platz 1
06099 Halle
ingrid.mertig@physik.uni-halle.de

Rossitza Pentcheva
Sektion Kristallographie
Geo- und Umweltwissenschaften
LMU München
Theresienstr. 41
80333 München
pentcheva@lrz.uni-muenchen.de

Overview of Invited Talks and Sessions

(lecture room A 151; Poster F)

Invited Talks

SYNF 2.1	Tue	14:30–15:00	A 151	**Tunable two-dimensional electron gases in correlated electronic systems** — •J. Mannhart, G. Hammerl, T. Kopp, C. Richter, C.W. Schneider, S. Thiel, N. Reyren, A.D. Caviglia, S. Gariglio, D. Jaccard, J.-M. Triscone, L. Fitting-Kourkoutis, D. Muller, C. Cheng, J. Levy
SYNF 2.2	Tue	15:00–15:30	A 151	**New physics from electron correlations at oxide interfaces** — •Warren E. Pickett, Rossitza Pentcheva
SYNF 2.3	Tue	15:30–16:00	A 151	**Gigantic magnetoelectic responses in hellimagnets** — •Y. Tokura
SYNF 2.4	Tue	16:00–16:30	A 151	**Electrical field control of ferromagnets using multiferroics** — •Ramamoorthy Ramesh
SYNF 2.5	Tue	16:30–17:00	A 151	**Spintronics with multiferroic materials** — •Agnes Barthelemy
SYNF 2.6	Tue	17:00–17:30	A 151	**Magnetoelectric effects at multiferroic interfaces** — •Evgeny Tsymbal

Sessions

SYNF 1.1–1.11	Tue	10:30–13:15	A 151	**Ferroic materials and novel functionalities I**
SYNF 2.1–2.6	Tue	14:30–17:30	A 151	**Ferroic materials and novel functionalities II**
SYNF 3.1–3.3	Tue	18:30–19:30	Poster F	**Ferroic materials and novel functionalities III - Poster (joined by O posters)**

SYNF 1: Ferroic materials and novel functionalities I

Time: Tuesday 10:30–13:15 Location: A 151

SYNF 1.1 Tue 10:30 A 151

Characterization of ultra thin epitaxial $BaTiO_3$ films on Pt(111): A LEED, STM and XPS study — •Stefan Förster and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle

Ultra thin epitaxial $BaTiO_3$ films have been grown on a Pt(111) single crystal substrate by r.f. magnetron sputtering and characterized by LEED, STM and XPS. The $BaTiO_3$ films were deposited at room temperature under a pressure of about $2.5{\cdot}10^{-3}$ mbar of Argon (80 %) and Oxygen (20 %) gas mixture and subsequently annealed in UHV. The magnetron sputtered films exhibit a high reproducibility of film thickness and composition. XPS spectra of the films are in good agreement with spectra of a $BaTiO_3$(111) single crystal, indicating that the films grow with $BaTiO_3$ stoichiometry. The weakening of the XPS signal from the Pt substrate was used to estimate the film thickness in the range up to several nm. Annealing to temperatures above 900 K leads to highly ordered films which are stable up to 1250 K. Their LEED pattern show several different structures depending on the preparation conditions which includes the $(\sqrt{3} \times \sqrt{3})$ structure known from the $BaTiO_3$(111) single crystal surface. Atomically resolved STM images confirm the $\sqrt{3}$ structure. Additionally, they show the growth of extended flat islands with diameters up to 200 nm separated by steps of multiple unit cell heights. These $BaTiO_3$ films might be ideal playground for future investigations of multiferroic systems.

SYNF 1.2 Tue 10:45 A 151

Exchange bias coupling in La0.7Sr0.3MnO3/BiFeO3 heterostructures — •Mark Huijben, Ying-Hao Chu, Lane W. Martin, Jan Seidel, Nina Balke, Martin Gajek, Chan-Ho Yang, Pu Yu, Micky Holcomb, and Ramamoorthy Ramesh — Department of Physics & Department of Materials Science and Engineering, University of California, Berkeley, USA

Heterostructures based on perovskite transition-metal oxides have attracted much attention because of the possibility of tuning the magnetic and electronic properties of thin films through interface effects such as exchange interactions, charge transfer, and epitaxial strain. The development and understanding of multiferroic materials such as BiFeO3, have piqued the interest with the promise of coupling between order parameters such as ferroelectricity and antiferromagnetism. In this study we investigate the magnetic properties in ferromagnetic-antiferromagnetic multiferroic heterostructures by using atomic scale controlled growth through laser-MBE in combination with real-time RHEED monitoring. We will show the controlled coupling at the interfaces in La0.7Sr0.3MnO3/BiFeO3 heterostructures. This coupling behavior is investigated by structural measurements, such as x-ray reciprocal space mapping to clarify strained states, and magnetic measurements to gain a deeper fundamental understanding of the interactions at these interfaces. The interface coupling displays a strong enhancement in the coercivity of the La0.7Sr0.3MnO3 layer and a large shift in the magnetization hysteresis loops, indicating the existence of exchange bias coupling.

SYNF 1.3 Tue 11:00 A 151

electronic structure induced reconstruction and magnetic ordering at the LaAlO3/SrTiO3 interface — •zhingcheng zhong and paul kelly — Faculty of Science and Technology and MESA+ institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

The finding of a high mobility electron gas at the interface between two large band gap insulators LaAlO3 and SrTiO3 led to the observation of interface magnetic ordering and, more recently superconductivity. We study this interface using density functional theory (LDA and LDA+U), taking into account the possibility of interface structural relaxation, charge and spin ordering. We find that charge, orbital and magnetic ordering can occur in a quarter-filled band system. The lowest energy configuration is a charge-ordered antiferromagnetic insulator. At a slightly higher energy, we find a charge-ordered ferromagnetic insulator with a smaller band gap. We discuss various scenarios for explaining the experimental observations.

SYNF 1.4 Tue 11:15 A 151

Influence of polarization on the surface relaxation of perovskite ferroelectrics — •Michael Fechner, Ostanin Sergey, and Ingrid Mertig — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany

Ferroelectric materials exhibit a electric polarization which is spontaneous and switchable by an electric field. These materials become important due to their possible application in multiferroic materials. In our study we investigate clean (001) surfaces of FE perovskites from first principles. We consider three different systems which are $SrTiO_3$, BaTiO3, and PbTiO3. These compounds differ in their size of spontaneous polarization from zero ($SrTiO_3$) to moderate ($BaTiO_3$) to high values ($PbTiO_3$). Due to this we could investigate the surface relaxation and electronic properties with respect to the size and the direction of the spontaneous polarization. Latter is done by considering the cases of a polarization direction parallel and antiparallel to the surface normal. In our study it turns out that the direction of polarization at the surface is independently of the polarization in the lower lying layers and the considered material. The results of our study are in good agreement with recent experimental findings [1].

[1] Y. Urakami Ferroelectrics, 346 (2007)

SYNF 1.5 Tue 11:30 A 151

Dynamic strain in metallic vs insulating manganite films — •Martina Cornelia Dekker, Steffen Oswald, Ludwig Schultz, and Kathrin Doerr — IFW Dresden, Germany

The use of a ferro- and piezoelectric substrate, PMN-PT (001) $(PbMg_{1/3}Nb_{2/3}O_3)_{0.72}(PbTiO_3)_{0.28}$, allows us to biaxially compress as grown epitaxial films by as much as 0.2% [1]. This reversible dynamic strain process gives a unique insight into the effect of strain on perovskite oxides, eliminating effects such as varying oxygen concentration, which may occur when several substrates with different lattice mismatch are used.

We have prepared PLCMO $(Pr_{1-x}La_x)_{0.7}Ca_{0.3}MnO_3$ films on PMN-PT substrates for a range of x values. Around $x = 0.6$, the system exhibits a transition from an insulating to a metallic ground state. We have recorded changes in magnetic moment and transition temperature upon varying x, and compared the effects of dynamic strain on transport behaviour in the metallic and insulating ground states.

[1] C. Thiele et al., Phys. Rev. B 75, 054408 (2007)

SYNF 1.6 Tue 11:45 A 151

Strain-dependent magnetism and electric transport properties of $La_{0.7}Sr_{0.3}CoO_3$ films — •Andreas Herklotz, Diana Rata, Orkidia Bilani, Ludwig Schultz, and Kathrin Dörr — IFW-Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

The electronic and magnetic properties of some perovskite-type 3d transition metal oxides are known to be sensitive to epitaxial strain. In order to investigate the influence of strain in $La_{0.7}Sr_{0.3}CoO_3$ (LSCO) compound, epitaxial films under different biaxial strain have been grown using various substrates. Additionally, piezoelectric substrates of the composition $0.72PbMg_{1/3}Nb_{2/3}O_3$-$0.28PbTiO_3$ (PMN-28%PT) were employed to control the in-plane strain dynamically by applying an electrical field. An insulator-type behaviour was observed in films grown under tensile strain, whereas compressed films show bulk, metallic properties. This drastic influence of strain was confirmed by using the PMN-PT substrates, where a reversible strain of 0.15% caused a resistance change of one order of magnitude at room temperature. On the contrary, the magnetization data revealed a rather small impact of tensile strain on the magnetic behaviour of LSCO films. We suggest that the insulator state of $La_{0.7}Sr_{0.3}CoO_3$ is caused by a stain-induced static Jahn-Teller-type deformation of the CoO_6 units, which may be efficient as a localization mechanism.

SYNF 1.7 Tue 12:00 A 151

Separation of magnetic and dielectric domains in $BiFeO_3$ and $BiCrO_3$ thin films — •Denny Köhler[1], Ulrich Zerweck[1], Christian Loppacher[3], Stephan Geprägs[2], Sebastian Gönnenwein[2], Rudolf Gross[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Walter-Meissner Institut, Bayrische Akademie der Wissenschaften, München — [3]Laboratoire de Matériaux et Microélectronique de Provence, Universités Paul Cézanne, Marseille

In our work we present low-temperature noncontact-AFM investigations (nc-AFM) in combination with Kelvin Probe Force Microscopy (KPFM) and Magnetic Force Microscopy (MFM) to investigate the magnetic and ferroelectric properties of $BiFeO_3$ and $BiCrO_3$ thin films on the nm length scale. Samples are prepared as described in [1]. Complementary to nc-AFM measurements, Piezoresponse Force Microscopy (PFM) was used to deduce the ferroelectric polarisation of the investigated thin films.

Our experiments show that the separation of magnetic and electrostatic forces is possible by simultaneously running KPFM and MFM, but delicate due to the fact that both interactions are of long range nature. We show the separation of ferroelectric and magnetic domains on both materials and monitored a magnetic phase transition on $BiCrO_3$.

[1] S. Geprägs et al., *Phil. Mag. Lett.* **87**: 141-147 (2007)

SYNF 1.8 Tue 12:15 A 151

Contrast Mechanism for the Detection of Ferroelectric Domains on all Faces of LiNbO3 using Piezoresponse Force Microscopy — Tobias Jungk, Akos Hoffmann, and •Elisabeth Soergel — Institute of Physics, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

We apply piezoresponse force microscopy (PFM) to reveal the domain structures on all faces of LiNbO3 single crystals. Therefore we investigated a two-dimensionally poled sample, all faces optically polished. On the z-face the PFM contrast is known to be caused by the piezoelectrically driven thickness change of the crystal. On the x- and y- faces, however, the contrast mechanism was found to be governed by a lateral movement of the surface underneath the tip. Depending on the relative orientation of the cantilever with respect to the crystallographic axes of the sample this results in a torsion or buckling movement of the cantilever. In order to support this explanation we mounted the sample on a high-precision rotation stage. The high stability of the set-up allows to rotate the sample during data acquisition. We could therefore precisely determine the angular dependency of the movement on the tip on the crystallographic axis. The experimental results are in good agreement with the theoretically expected values.

Acknowledgments: Financial support of the DFG research unit 557 and of the Deutsche Telekom AG is gratefully acknowledged.

SYNF 1.9 Tue 12:30 A 151

All-electron calculations of electronic tunneling in perovskite magnetic tunnel junctions — •Daniel Wortmann and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

Combining materials with different ferroic orders into a single multilayer transport junction offers the prospect of novel devices like 4-bit memory cells or switching schemes based on the coupling between the different ferroic configurations. However, the materials used in such junctions often exhibit extremely complex interrelations between details of their atomic, electronic and magnetic structure making the simulation of such multilayer junctions on an *ab initio* level a necessity for any realistic setup but a true challenge at the same time. We will present calculations using our all-electron, full-potential transport code [1] based on the embedding Green function method. For the model setup of a $SrRuO_3/SrTiO_3/SrRuO_3$ tunneljunction we calculate the spin-polarized electronic tunnel-current and investigate the effects of lattice distortions on the orbital character of the current carrying Bloch states in $SrRuO_3$ and the resulting changes on the spin-polarization of the current.

[1] D. Wortmann, H. Ishida, and S. Blügel, Phys. Rev. B **66**, 075113 (2002).

SYNF 1.10 Tue 12:45 A 151

Ferroelectric Tunnel Junctions — •Hermann Kohlstedt[1], Nicholay Pertsev[2], Adrian Petraru[1], Ulrich Poppe[1], and Rainer Waser[1] — [1]Institut für Festkörperforschung and CNI, Forschungszentrum Jülich, Jülich, Germany — [2]A. F. Ioffe Physico-Technical Institute, St. Petersburg, Russia

Quantum mechanical electron tunneling through nanoscale ferroelectric barriers is discussed for symmetric (identical electrodes) and asymmetric (dissimilar electrodes) junctions. It is shown that the lattice strains of piezoelectric origin modify the I-V relationship owing to strain-induced changes of the barrier thickness, electron effective mass, and position of the conduction-band edge. The effect of internal electric field caused by incomplete screening of polarization charges at the surfaces of a ferroelectric barrier is analyzed. For asymmetric junctions, this depolarizing-field effect also leads to a considerable change of the barrier resistance after the polarization reversal. The crossover between two types of hysteretic behavior is described taking into account both the strain and depolarizing-field effects. The results already obtained for these new types of tunnel junctions and the theoretical and experimental challenges existing in this area will be discussed. Experiments on the scaling properties of ultra-thin wedged BaTiO3 films will be presented. At the end we will provide an overview for the current status of the international studies of the so-called multiferroic tunnel junctions. By combing ferroelectric or multiferroic tunnel barriers with ferromagnetic and/or superconducting electrodes, a whole *zoo* of novel tunnel junctions can be proposed.

SYNF 1.11 Tue 13:00 A 151

Resistive memory switching in perovskite-derivative single crystals — •P. Müller[1], F. Chowdhury[1], V. Dremov[1], Y. Koval[1], F. Lichtenberg[2], S. Müller[3], D. Schmeisser[3], and R. Pentcheva[4] — [1]Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg — [2]Experimentalphysik VI, Universität Augsburg — [3]Lehrstuhl Angewandte Physik-Sensorik, BTU Cottbus — [4]Department of Earth and Environmental Sciences, LMU München

We investigated several layered perovskite derivatives of the family $A_nB_nO_{3n+2}$, such as $LaTiO_{3.41}$, $CaNbO_{3.41}$ and $SrNbO_{3.41}$, which can be considered as a stacking of blocks consisting of 5 perovskite layers. Electric transport across these layers takes place via intrinsic tunnelling. Mesa devices with a cross-sectional area of 50 to 200 μm^2 and a height between 30 and 500 nm were fabricated by electron-beam lithography and ion-beam etching. Both dc I-V characteristics and pulsed current injection have shown switching between different resistive states in these materials. The resistive states have long-term stability, which makes them interesting for memory applications. The transport experiments suggest that switching and resistive memory are controlled by trapping and release of charge carriers. Furthermore, photoelectron and NEXAFS spectroscopy of cleaved $LaTiO_{3.41}$ surfaces have been performed. The results are compared to recent correlated band theory (LDA+U) calculations.

SYNF 2: Ferroic materials and novel functionalities II

Time: Tuesday 14:30–17:30 Location: A 151

Invited Talk SYNF 2.1 Tue 14:30 A 151

Tunable two-dimensional electron gases in correlated electronic systems — •J. Mannhart[1], G. Hammerl[1], T. Kopp[1], C. Richter[1], C.W. Schneider[1], S. Thiel[1], N. Reyren[2], A.D. Caviglia[2], S. Gariglio[2], D. Jaccard[2], J.-M. Triscone[2], L. Fitting-Kourkoutis[3], D. Muller[3], C. Cheng[4], and J. Levy[4] — [1]Center for Electronic Correlations and Magnetism, Augsburg University, Germany — [2]University of Geneva, Switzerland — [3]Cornell University, USA — [4]University of Pittsburgh, USA

The unique properties of two-dimensional electron gases in semiconductor heterostructures provide the basis for a variety of high-performance devices, such as high electron mobility transistors or quantum well lasers, and for fundamental phenomena, such as the integer and fractional quantum Hall effects. Because standard semiconductors are mean-field systems it is intriguing that recent progress in heterostructure growth of oxides offers now the possibility to fabricate two-dimensional gases of materials with interacting electrons. These electronic correlations shape the properties of the electron gas, which, for example, may develop a ferromagnetic or a superconducting ground state. In field-effect transistor configurations these electron gases can be tuned [1], so that for example switchable, transparent superconductors are obtained [2]. In the presentation I will provide an overview of our experiments with such electron systems.

[1] S. Thiel et al., Science 313, 1942 (2006)
[2] N. Reyren et al., Science 317, 1196 (2007)

Invited Talk SYNF 2.2 Tue 15:00 A 151

New physics from electron correlations at oxide interfaces — •Warren E. Pickett[1] and Rossitza Pentcheva[2] — [1]Department of Physics, University of California, Davis, California 95616, USA — [2]Department of Earth and Environmental Sciences, University of Munich, Theresienstrasse 41, 80333 Munich, Germany

Disruption of periodic order in ionic materials (simplest examples are flat surfaces and abrupt heterointerfaces) often entail "charge mismatch" and polar layers. The strength of Coulomb forces dictates that the mismatch be accommodated within a few atomic distances. A mechanism in which the mismatch can be neutralized within a single atomic layer – strong intra-atomic repulsion resulting in charge order – will be discussed, with examples taken from ab initio calculations of abrutp LAO/STO and LTO/STO (001) heterointerfaces. The properties (conductivity, magnetism) of the interface can be dependent on atomic relaxation and of defects (oxygen vacancies, cation exchange, etc.). The "new materials " aspects of short-period multilayers will also be discussed.

Invited Talk SYNF 2.3 Tue 15:30 A 151

Gigantic magnetoelectic responses in hellimagnets — •Y. Tokura — Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan

Multiferroics, the materials in which both (anti)ferromagnetism and ferroelectricity can coexist, are the prospective candidate which can potentially host the gigantic magnetoelectric (ME) effect. A useful hint to designing of the strong magnetoelectric coupling has been gained by the recent discovery of the ferroelectricity in the transverse-spiral magnets, such as perovskite manganites. The multiferroics based on the spin-current (or inverse Dzyaloshinskiy-Moriya interaction) mechanism has recently been realized also in the conical spin state of chromite spinels where the transverse spiral component coexists with the uniform magnetization component along the cone axis. In those compounds, the clamping between the magnetic and ferroelectric domains can show up, perhaps enabling the magnetic (electric) control of the ferroelectric (ferromagnetic) domains. Multiferroics with the strong ME correlation may also provide a unique arena to test new optical effects. This includes the so-called magnetization-induced second harmonic generation (MSHG) and the nonreciprocal dichroism dependent on the light propagation direction (but not on the light polarization), termed the optical magnetoelectric (OME) effect as well as the electrically driven spin excitations like electromagnons. We present the late advances in our study of exploring such hellimagnets (screw, cycloidal, and conical magnets) as showing strong ME coupling and novel optical responses.

Invited Talk SYNF 2.4 Tue 16:00 A 151

Electrical field control of ferromagnets using multiferroics — •Ramamoorthy Ramesh — Dept. of Materials Science and Engineering and Dept. of Physics, University of California, Berkeley, CA 94720

Complex perovskite oxides exhibit a rich spectrum of functional responses, including magnetism, ferroelectricity, highly correlated electron behavior, superconductivity, etc. The basic materials physics of such materials provide the ideal playground for interdisciplinary scientific exploration. Over the past decade we have been exploring the science of such materials (for example, colossal magnetoresistance, ferroelectricity, etc) in thin film form by creating epitaxial heterostructures and nanostructures. Among the large number of materials systems, there exists a small set of materials which exhibit multiple order parameters; these are known as multiferroics. Our goal is to be able to deterministically control the state of a ferromagnet with the application of an electric field, by using heterostructures that include multiferroic perovskites. Our model multiferroic is BiFeO3, which ahs ferroelectric and antiferromagnetic order well about room temperature. Our work so far has shown that the AFM order can be controlled through coupling with the ferroelectricity. The next step is to explore the coupling of a ferromagnet to this antiferromagnet through the exchange biasing concept. Ultimately, this will give us the opportunity to switch the state of a ferromagnet (and therefore the spin polarization direction) by simply applying an electric field to the underlying antiferromagnetic ferroelectric. In this talk, I will describe our progress to date on this exciting possibility.

Invited Talk SYNF 2.5 Tue 16:30 A 151

Spintronics with multiferroic materials — •Agnes Barthelemy — Unite Mixte de Physique CNRS/Thales and Universite Paris-Sud, Route de partementale 128, 91767 Palaiseau, France

Multiferroics are singular materials that can exhibit simultaneously electric and magnetic orders. Some are ferroelectric and ferromagnetic and provide the opportunity to encode information in electric polarization and magnetization to obtain four logic states. However, such materials are rare and schemes allowing a simple electrical readout of these states have not been demonstrated in the same device. Here, we show that films of La0.1Bi0.9MnO3 (LBMO) are ferromagnetic and ferroelectric, and retain both ferroic properties down to a thickness of 2 nm. We have integrated such ultrathin multiferroic films as barriers in spin-filter-type tunnel junctions that exploit the magnetic and ferroelectric degrees of freedom of LBMO.Whereas ferromagnetism permits read operations reminiscent of magnetic random access memories (MRAM), the electrical switching evokes a ferroelectric RAM write operation. Significantly, our device does not require the destructive ferroelectric readout, and therefore represents an advance over the original four-statememory concept based on multiferroics.

Invited Talk SYNF 2.6 Tue 17:00 A 151

Magnetoelectric effects at multiferroic interfaces — •Evgeny Tsymbal — Department of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588, USA

Multiferroic materials have recently attracted significant interest due to the coupling between different order parameters that can lead to new functionalities. One of the promising ways to achieve a strong coupling is to use heterogeneous interfaces, producing lattice strain, chemical bonding, and charge transfer effects, not existing in the bulk phase. For example, magnetoelectric effects may strongly be enhanced at the ferromagnetic/ferroelectric interfaces where the influence of ferroelectric displacements on the interface electronic structure may lead to a change in the magnetic moment and magnetic anisotropy. Ferromagnet/ferroelectric interfaces are also promising for application in ferroelectric tunnel junctions where a thin-film ferroelectric is used as a barrier layer. In these junctions, ferroelectric polarization reversal may lead to a sizable change in the conductance and the spin polarization. This talk will address our recent progress in the theoretical studies of these multiferroic interfaces and tunnel junctions which are interesting for application in multifunctional electronic devices.

SYNF 3: Ferroic materials and novel functionalities III - Poster (joined by O posters)

Time: Tuesday 18:30–19:30 Location: Poster F

SYNF 3.1 Tue 18:30 Poster F

La and Mn co-doping effects on the structure and electrical properties of $BiFeO_3$ thin films — •Abdelilah Lahmar[1], Giray Kartopu[1], Salah Habouti[1], Claus-Henning Solterbeck[1], Mohammed Es-Souni[1], Brahim Elouadi[2], and Michel Couzi[3] — [1]Institute for Materials and Surface Technology, University of Applied Sciences Kiel, Germany — [2]Université de La Rochelle, Department de Chimie, La Rochelle, France — [3]Laboratoire de Physico-Chimie Moléculaire, CNRS, Université Bordeaux, Talence, France

The structural, electric, and magnetic properties of the solid solution $Bi_{1-x}La_xFe_{1-x}Mn_xO_3$ ($0 \leq x \leq 0.1$) have been investigated. Thin films have been grown by a sol-gel spin-coating method on (111)Pt/Ti/SiO_2/Si substrates. The incorporation of both (La^{3+}, Mn^{3+}) cations in bismuth ferrite host lattice was found to improve dielectric, ferroelectric, and magnetic properties. A comparative study of 5%La-, 5%Mn-, and 5%LaMn- doped $BiFeO_3$ has been undertaken with the aim of understanding the role of each doping element on the structure and electrical properties. Raman spectroscopy has been used for a detailed structural characterization, and the results obtained are compatible with our ferroelectric investigations.

SYNF 3.2 Tue 18:30 Poster F

HX-PES study of $LaAlO_3/SrTiO_3$ heterostructures — •Götz Berner[1], Andreas Müller[1], Stefan Thiel[2], Christof

Schneider[2], Michael Sing[1], Jochen Mannhart[2], and Ralph Claessen[1] — [1]Experimentelle Physik IV, Universität Würzburg — [2]Experimentelle Physik VI, Universität Augsburg

Oxide heterostructures are of special interest due to the unexpected new physics occurring at the interface. E.g., a quasi-two-dimensional electron gas (2DEG), which even becomes superconducting at lowest temperatures forms at the interface of the two band insulators $LaAlO_3/SrTiO_3$, if at least 4 unit cells of $LaAlO_3$ are grown on TiO_2 terminated $SrTiO_3$.

In principle, angle dependent hard x-ray photoemission spectroscopy (HX-PES) is a powerful tool to get insight in both the change in chemical state and the vertical distribution of the additional charge at the interface by probing the intensity ratio of the Ti^{3+} 2p and Ti^{4+} 2p core lines. However, first measurements surprisingly did not show any Ti^{3+} 2p signal for various detection angles. This is in sharp contrast to the expectation from simple electrostatic considerations and recent estimates from SXRD measurements. Both claim an area carrier density corresponding to 0.5 electron per unit cell. In contrast, our HX-PES measurements indicate a much lower carrier concentration consistent with Hall measurements on our samples. As possible explanation for these discrepancies we discuss the effects of the finite $LaAlO_3$ thickness and the oxygen defects at the interface.

SYNF 3.3 Tue 18:30 Poster F

Hybrid-functional applied to a model ferroelectric: $SrTiO_3$ — •Roman Wahl — University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The structural, electronic and phonon properties of the cubic and tetragonal phase of $SrTiO_3$ are studied from *ab initio*. The calculations are performed in the pseudopotential DFT framework using the local density approximation (LDA), gradient corrected functionals (PBE, PBEsol) and hybrid functionals (HSE03) as implemented in the Vienna ab initio simulation package (VASP). Due to the large variation of theoretical predictions for the frequency of the F_{1u} (Γ_{15}) zone-center phonon mode ($100i$ - 64 cm^{-1}) special attention is put on this particular mode and its volume dependency.