International workshop on Nanoferronics:

"Novel multifunctional metal-oxide tunnel-junctions relevant for future devices"

Aachen, October 9-10, 2008

Scientific Coordinators:

Marjana Ležaić (Forschungszentrum Jülich, Germany)

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Summary

The acronym *nanoferronics* stands for spin transport electronics through multifunctional (multiferroic) tunnel junctions. The motivation for the workshop was to discuss, explore and trigger the next steps in this rapidly developing field.

Last December, the prestigious scientific journal *Science*, classified recent advances on multiferroics and oxide interfaces as one of the 10 breakthroughs of the year! It is easy to see why the oxide junctions attract so much attention by considering just one example. In the past year, in several experiments conducted on the interface between two insulators, $SrTiO_3$ (STO) and $LaAlO_3$ (LAO), this interface was found to exhibit a whole spectrum of different behaviors, ranging from magnetism to superconductivity or to metal-insulator transition. The mentioned investigations at LAO/STO interface are just an example, and they result from sustained progress in the growth of complex oxides thin films using advanced deposition techniques during the past two decades. Combined with sophisticated real time in-situ monitoring of surface and structural properties, this opened new avenues to engineer complex oxides interfaces, heterostructures and devices at the atomic scale level. Such interfaces and the variety of different physical phenomena that are observed at them were one of the main topics of the workshop.

During the invited talks and the poster session the discussions went along several directions. These include:

- The theoretical tools and the results of the Density Functional Theory applied on oxides and their junctions
- The discussion of observed phenomena at the interfaces of perovskite materials
- The development of experimental tools relevant for the characterization of oxide films and interfaces
- The control and manipulation of the spin-dependent quantum transport through the tunnel junctions e.g. by external magnetic or electrical fields
- The switching of the magnetization and the ferroelectric polarization as relevant for reading and writing of information.

PROGRAM

Thursday, October 9

	Welcome
09.00 - 10.40	**Session 1 : Current status and trends** *Discussion leader: Wolfgang Kleemann*
9:00	**Hans Schmid, Universite de Genèva, Switzerland** **The trail from Pierre Curie to maximal single phase multiferroic complexity**
9:50	**Nicola Spaldin, University of California, Santa Barbara, USA** **Recent progress in single phase multiferroics**
10.40	Coffee break
11:00 - 13:00	**Session 2 : Ferroelectricity and magnetism** *Discussion leader: Marjana Ležaić*
11:00	**Philippe Ghosez, University of Liege, Belgium** **Engineering exotic phenomena at ferroelectric oxide interfaces : a first-principles perspective**
11:40	**Gustav Bihlmayer, Forschungszentrum Jülich, Germany** **Describing complex magnetism from first principles**
12:20	**Claude Ederer, Trinity College Dublin, Ireland** **Toroidal moments and magneto-electric coupling: the case of $BiFeO_3$ versus $FeTiO_3$**
13:00 - 14:30	Lunch Break
14:30 - 16:30	**Session 3 : Oxides and interfaces** *Discussion leader: Liu-Hao Tjeng*
14:30	**Yasuyuki Hikita, University of Tokyo, Japan** **Controlling Band Offsets in Manganite-Titanate Heterojunctions**
15:10	**Alexander Brinkman, University of Twente, Enschede, Netherlands** **Magnetoresistance oscillations and relaxation effects at the $SrTiO_3$-$LaAlO_3$**
15:50	**Andrea Caviglia, University of Geneva, Switzerland** **Electric Field Control of the $LaAlO_3$/$SrTiO_3$ Interface Ground State**
16:30 - 16:50	Coffee break
16:50 - 18:10	**Session 4 : Correlations at interfaces I** *Discussion leader: Silvia Picozzi*
16:50	**Ansgar Liebsch, Forschungszentrum Jülich, Germany** **Coulomb correlations at surfaces and interfaces**
17:30	**Warren E. Pickett, University of California Davis, USA** **Surface-Interface Coupling of $LaAlO_3$ overlayers on $SrTiO_3$: Domestication of the Polar Catastrophe**
18:40	Poster session / Dinner

Friday, October 10

09:00 - 11:00	**Session 5 : Advanced Analytics** *Discussion leader: Uwe Klemradt*
09:00	**Salia Cherifi, Institut Néel, CNRS, Grenoble, Fance** **Imaging submicron ferroelectric domains with slow electrons**
09:40	**Chunlin Jia, Forschungszentrum Jülich, Germany** **Atomic-scale study of electric dipoles near 180^0 domain walls in ferroelectric thin films**
10:20	**Bernhard Keimer, MPI for Solid State Research, Stuttgart, Germany** **Spectroscopy of electronic reconstructions at oxide interfaces**
11:00 - 11:30	Coffee break
11:30 - 13:30	**Session 6 : Correlations at interfaces II** *Discussion leader: Stefan Blügel*
11:30	**Kiyoyuki Terakura, JAIST, Ishikawa, Japan** **Screening mechanism for polar discontinuity for $LaAlO_3/SrTiO_3$ thin films**
12:10	**Zhicheng Zhong, University of Twente, Netherlands** **Electronic structure induced reconstruction and magnetic ordering at the $LaAlO_3/SrTiO_3$ interface**
12:50	**Evgeny Tsymbal, University of Nebraska-Lincoln, Lincoln, USA** **Modeling of Magnetoelectric Interfaces**
13:30 - 15:00	Lunch Break
15.00 - 17:00	**Session 7 : Strain-assisted phenomena** *Discussion leader: Thomas Brückel*
15:00	**Nikolay. A. Pertsev, Physico-Technical Institute, St. Petersburg, Russian Federation** **Strain-mediated electric effects in ferroic heterostructures and tunnel junctions**
15:40	**Darrell G. Schlom, Cornell University, USA** **The effect of strain on thin ferroelectric and multiferroic layers**
16:20	**Sebastian Gönnenwein, Bayrische Akademie der Wissenschaft, Garching, Germany** **Magnetoelastic magnetization manipulation in ferromagnet/ferroelectric hybrids**
17:00 - 17:30	Coffee break
17:30 - 19:30	**Session 8 : Towards Oxide Electronics** *Discussion leader: Hermann H. Kohlstedt*
17:30	**Angès Barthélémy, Unité Mixte de Physique CNRS/Thales, Palaiseau, France** **Oxide based heterostructures for spintronics**
18:10	**Andreas Schmehl, University Augsburg, Germany** **EuO_{1-x} - A Half-Metallic Ferromagnetic Semiconductor with High Potential for Application Driven Science**
18:50	**Regina Dittmann, Forschungszentrum Jülich, Germany** **Influence of strain relaxation and interface configuration on the dielectric response of ferroelectric BST thin film capacitors**
20:00	Closing & Dinner

Poster contributions

Con-01 **Theo A. Costi**
Kondo Proximity Effect: How Does a Metal Penetrate Into a Mott Insulator?

Con-02 **Bruce A. Davidson**
Ferromagnetic correlations at atomically-engineered manganite interfaces

Con-03 **Mario Disch**
Probing ferroelectricity in ultrathin wedged epitaxial $BaTiO_3$ films

Con-04 **Michael Fechner**
Magnetic phase transition in two-phase multiferroics predicted from first principles

Con-05 **Christoph Friedrich**
All-Electron *GW* Calculations for Strontium and Barium Titanate

Con-06 **Vincent Garcia**
Magnetic tunnel junctions with ferroelectric tunnel barriers : electroresistance and tunneling magnetoresistance

Con-07 **Fumiyuki Ishii**
Noncollinear Magnetism in the Perovskite Manganite Superlattice

Con-08 **Hermann Kohlstedt**
A novel total electron yield set-up for interface studies under soft x-ray radiation and a simultaneously applied bias field

Con-09 **Alexey Melnikov**
Non-equilibrium surface and bulk spin-dynamics at Gd(0001)

Con-10 **Frederico D. Novaes**
Tunneling across a ferroelectric barrier : a first-principles study

Con-11 **Kourosh Rahmanizadeh**
First-principles investigation of thin $ATiO_3$ films with stacking faults

Con-12 **Hasan Sadat Nabi**
Microscopic origin of magnetism in hematite - ilmenite heterostructures

Con-13 **Marco Salluzzo**
XAS and XMCD spectroscopy on $Nd_1Ba_2Cu_3O_7$ /STO interface

Con-14 **Keisuke Shibuya**
Correlation between stacking defect and resistive switching in Sr_2TiO_4 thin films

Con-15 **Kunihiko Yamauchi**
Theoretical study of $La_{1-x}Sr_xMnO_3/BiFeO_3$ heterojunction: Exchange bias and magnetoelectric coupling

Con-16 **Wolfgang Kleemann**
$(Sr,Mn)TiO_3$ - a magnetoelectric multiglass

Con-17 **Marjana Ležaić**
Double perovskite multiferroics: the room temperature challenge

Con-18 **Mohammed Bouhassoune**
Electronic structure and effective masses in strained Silicon

Con-19 **Ersoy Sasioglu**
Ab initio many-body calculation of magnetic excitations in 3d transition metals

THE TRAIL FROM PIERRE CURIE TO MAXIMAL SINGLE PHASE MULTIFERROIC COMPLEXITY
NanoFerronics-2008
AT JUELICH

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We can distinguish today four so-called *primary ferroic* properties in crystals: ferromagnetic, ferroelectric, ferroelastic and ferrotoroidic (in historical order of "birth"). If two or more of them occur in the same phase, we speak of *single phase multiferroics*. Current interest focuses particularly on magnetoelectric multiferroics, but in many papers the term 'magnetoelectric' is often used in an ill-defined way and / or is confounded with 'multiferroic'. With terms such as 'magnetoelectric coupling' the situation is also often only vaguely described. We shall therefore put accent on symmetry considerations, which allow to foresee what is possible and what is not, and trace back the development, starting with Pierre Curie's conjecture that "materials should exist getting polarized by a magnetic field and magnetized by an electric field".

By combining thermodynamics with symmetry considerations, the point groups allowing crystallo-physical effects, such as linear and bilinear magnetoelectric effects can be evaluated.

Ferroic and multiferroic domains, their patterns and (coupled) switching can be understood by Aizu's system of the group / subgroup classification of phase transitions, allowing also to distinguish between full, partial or no coupling of order parameters during switching, without needing Landau theory. This system has recently been extended to ferrotoroidic crystals[1)].

The presence of ferroelasticity is found to be indispensable for coupled "reorientation switching" of the magnetic order parameters (by angles other than 180 deg.) by electric and magnetic fields or by stress. Shortcomings resulting from this fact will be discussed.

Ferrotoroidic domains are spatially identical either with ferromagnetic domains or with antiferromagnetic ones and depending on symmetry can in principle be time-reversed by a magnetic field or magnetoelectrically by crossed or collinear electric and magnetic fields[2)].

Examples of ferrotoroidic domains will be discussed for $Ga_{2-x}Fe_xO_3$, $LiCoPO_4$ and $Co_3B_7O_{13}I$. Recent neutron scattering data[3)] implying average monoclinic symmetry for the IC-antiferromagnetic /ferroelectric / ferroelastic phase of $BiFeO_3$, will also be explained.

Maximal multiferroic complexity occurs i) when all four primary ferroics are present, i.e., all possible crystallo-physical effects are allowed and ii) when the prototype symmetry is highest (cubic) and the ferroic phase symmetry lowest (triclinic), leading to a maximal number of possible domain states. This number may even be doubled if antiphase domains are allowed by symmetry.

1) Litvin D B, 2008 Ferroic classifications extended to ferrotoroidic crystals *Acta Crystallogr.* A **64** 316-20
2) Schmid H 2008 Some aspects of symmetry of ferroics and single phase multiferroics *Journal of Physics: Condensed Matter,* in press
3) Lebeugle D et al. Elecric field-induced spin-flop in $BiFeO_3$ single crystals at room temperature *Physical Review Letters* **100** 227602/1-/4

RECENT PROGRESS IN SINGLE PHASE MULTIFERROICS
NanoFerronics-2008
JUELICH

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The recent resurgence of interest in multiferroics combining ferromagnetism and ferroelectricity has led to the identification of new mechanisms for ferroelectricity that are compatible with the existence of magnetism. Here we provide a taxonomical classification of such ferroelectric mechanisms, and review the chemistry behind the structural or electronic driving forces that allow magnetism and ferroelectricity to occur simultaneously. In addition, we illustrate the utility of theoretical and computational materials methods in the understanding and design of multiferroic materials. Finally, we discuss an intriguing novel application of multiferroics: Testing the validity of promising theories of physics (supersymmetry, grand unification, etc.) beyond the standard model.

Engineering exotic phenomena at ferroelectric oxide interfaces : a first-principles perspective

Philippe Ghosez

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Thanks to recent advances in epitaxial oxide growth, ferroelectric oxide heterostructures and superlattices can nowadays be realized with atomic-level precision. This is bringing the field of ferroelectrics to an entirely new level and offers tremendous new possibilities for creating artificial multifunctional materials and devices [1]. First-principles calculations constitute a powerful tool to clarify the physics of oxide heterostructures at the atomic level and to guide the experimentalists toward the design of artificial nanostructures with enhanced or, eventually, totally new properties. After a brief introduction, I will focus on two concrete examples. In a first part, I will illustrate how it is possible to couple ferroelectric and antiferrodistortive structural instabilities at the inter-layer interfaces of $PbTiO_3$/$SrTiO_3$ superlattices in order to induce an *improper ferroelectric* behavior and obtain unusual dielectric properties of direct interest for technological applications [2]. In a second part, I will report recent first-principles results concerning ferroelectric tunnel junctions and deduce some general rules for the design of optimized structures.

Work done in collaboration with Eric Bousquet, Patrick Hermet, Daniel Bilc, Frederico Novaes, Matthew Dawber, Céline Lichtensteiger and Jean-Marc Triscone and supported by the FAME NoE, the MaCoMuFi Strep project and the VolkswagenStiftung.

[1] J. Junquera and Ph. Ghosez, “First-principles study of ferroelectric oxide epitaxial thin films and superlattices: role of the mechanical and electrical boundary conditions”, *J. Computational Theoretical Nanotechnology* **5**, 1 (2008) [http://xxx.lanl.gov/abs/0711.4201]

[2] E. Bousquet, M. Dawber, N. Stucki, C. Lichtensteiger, P. Hermet, S. Gariglio, J.-M. Triscone, and Ph. Ghosez, “Improper ferroelectricity in perovskite oxide artificial superlattices”, *Nature* **452**, 732-736 (2008)

Describing complex magnetism from first principles

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The investigation of multiferroic materials by ab-initio methods requires an accurate treatment of their complex, sometimes long-ranged spin-structures, the inclusion of spin-orbit coupling effects and, if necessary, to take into account the correlated nature of the d of f electrons of their constituent atoms. Together with the careful treatment of the electronic system, the ionic degrees of freedom have to be accurately captured. In the last years we could establish methods to describe the underlying interactions, i.e. the symmetric and antisymmetric exchange, the magnetocrystalline anisotropy and their dependence on dimensionality and structure in realistic materials. This talk will focus on low-dimensional magnetic systems and the importance of relativistic effects for the magnetic properties. We discuss the progress in density functional theory calculations for a quantitative description of structure and magnetism, which is at the heart of multiferroic materials.

Toroidal moments and magneto-electric coupling: the case of $BiFeO_3$ versus $FeTiO_3$

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The recent observaton of ferrotoroidic domains in $LiCoPO_4$ [1] has led to increased discussion of the importance of the concept of toroidal moments, in particular with respect to the role played by toroidal moments to mediate coupling between magnetic and ferroelectric order in multiferroic materials. A magnetic toroidal moment $\vec{T}$ represents a vector-like electromagnetic multipole moment that changes sign under both time and space inversion, and thus has the correct symmetry to couple the magnetization $\vec{M}$ and the electric polarization $\vec{P}$ via a trilinear free energy invariant of the form $\vec{T} \cdot \left(\vec{P} \times \vec{M} \right)$.

In this talk I will present both symmetry arguments and results of first principles density functional theory calculations, which show that the weak magnetic moment in the A-site magnetic compound $FeTiO_3$ is coupled to the electric polarization, whereas this is not the case in the isostructural multiferroic $BiFeO_3$ [2]. In addition, I will present a semi-quantitative analysis of the magnetic toroidal moments in both systems, which illustrates nicely the different magnetic symmetries of the two compounds, and hints at a crucial role played by the toroidal moment in mediating magnetoelectric coupling.

I will also illustrate the basic difficulties one encounters when attempting to evaluate the magnetic toroidal moment in a periodic system, and I will show how to overcome these difficulties in the limit of localized magnetic moments [3].

[1] B. B. Van Aken, J. P. Rivera, H. Schmid, and M. Fiebig, Nature 449 (2007).

[2] C. Ederer and C. J. Fennie, arXiv:0806.0589 (2008).

[3] C. Ederer and N. A. Spaldin, Phys. Rev. B 76, 214404 (2007).

Controlling Band Offsets in Manganite-Titanate Heterojunctions

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The band offset, defined as the energy level discontinuity between two materials at their juncture, is one of the crucial parameters when considering the electronic structure across a heterointerface. The band offsets determine the functional characteristics in diodes or transistors, and dominate the formation of artificial electronic states in quantum wells. With increasing numbers of reports on interface specific phenomena at oxide interfaces, a direct method of characterizing band offsets and techniques to manipulate them would enable further advance in designing functionalities in oxide electronics. In this talk, the main focus of our study is on the band offsets at Schottky interfaces between $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and Nb-doped $SrTiO_3$ (100) (NSTO), in which we present two different ways to manipulate the barrier heights. The first is barrier height tuning by external magnetic field in $La_{0.7}Sr_{0.3}MnO_{3-\delta}$/NSTO heterojunctions [1], reflecting strong magneto-orbital coupling in LSMO in proximity to the metal-insulator transition. The second is the control of the barrier heights by microscopic control of the interface termination, and hence the interface dipole arising from screening of the polarity mismatch at the interface. These two examples clearly demonstrate the significant role of the interface chemical bonds on the macroscopic behavior of the rectifying junction. In additional to conventional electrical probes, we have used internal photoemission spectroscopy to study the barrier heights [2]. This powerful technique allows direct measurement of the barrier height under applied magnetic field, and enables equilibrium measurements without application of a bias voltage.

[1] N. Nakagawa *et al.*, Appl. Phys. Lett. **86**, 082504 (2005).

[2] Y. Hikita *et al.*, Appl. Phys. Lett. **90**, 143507 (2007).

Magnetoresistance oscillations and relaxation effects at the $SrTiO_3$ – $LaAlO_3$ interface

M. van Zalk[1], J. Huijben[1], A.J.M. Giesbers[2], M. Huijben[1], U. Zeitler[2], J.C. Maan[2], W.G. van der Wiel[1], G. Rijnders[1], D.H.A. Blank[1], H. Hilgenkamp[1], and A. Brinkman[1]

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The discovery of conducting interfaces between the insulating perovskites $SrTiO_3$ and $LaAlO_3$ [1] has generated intensive research in recent years. The conduction arises from a charge redistribution that occurs at the interface in order to counteract an otherwise diverging electric potential in a polar material. So far, oxide interface samples exhibited metallicity, superconductivity below 200 mK and magnetic hysteresis below 300 mK [2]. Here we present transport measurements on $SrTiO_3$ — $LaAlO_3$ interfaces at 50 mK in magnetic fields up to 30 T [3]. The data provide insight in the nature of the magnetic phenomena and dimensionality of the transport. The hysteresis relaxes logarithmically as a function of time, suggestive of the presence of magnetic frustration. We observe magnetoresistance oscillations, which are periodic in $\sqrt{B}$, and not periodic in 1/B, as is the case for the well-known Shubnikov-de Haas oscillations. A possible relation with the formation of edge states on substrate terrace edges is discussed. The presence of such states would imply the existence of a highly mobile 2D electron gas at the interface.

[1] A. Ohtomo, H. Y. Hwang, Nature **427**, 423 (2004).

[2] A. Brinkman *et al.*, Nature Mater. **6**, 493 (2007).

[3] M. van Zalk *et al.*, cond-mat\0806.4450 (2008).

Electric Field Control of the $LaAlO_3/SrTiO_3$ Interface Ground State

A.D. Caviglia[1], N. Reyren[1], S. Gariglio[1], S. Thiel[2], D. Jaccard[1], T. Schneider[3], M. Gabay[4], J. Mannhart[2] and J.-M. Triscone[1]

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Electronic states with unusual properties can be promoted at interfaces between complex oxides. A particularly fascinating system is the interface between band insulators LaAlO3 and SrTiO3, which displays conductivity with high mobility. Recently two possible ground states have been experimentally identified: a magnetic state and a two dimensional (2D) superconducting condensate. In this contribution, field effect experiments performed on this system will be discussed. Using the electrostatic tuning of the carrier density, the phase diagram of the system has been explored, revealing a quantum phase transition (QPT) separating a 2D superconducting state from an insulating state. The critical exponents of the QPT are compatible with a 3D-XY model pointing at the key role of quantum phase fluctuations. The insulating phase displays signatures of weak localisation.

Coulomb correlations at surfaces and interfaces

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Heterostructures involving transition metal oxides are currently of great fundamental and practical interest. As a result of lattice, electron and orbital reconstruction new properties may occur that do not exist in bulk materials and that might lead to interesting appliactions. The hallmark of strongly correlated systems is their tremendoussensitivity to small changes of key parameters such as temperature, pressure, doping, and crystal field splitting. Here we review some of the typical modifications associated with surfaces and interfaces. Dynamical mean field theory is used to evaluate the effect of these changes on the electronic properties, in particular, in the vicinity of metal insulator transitions.

Surface-Interface Coupling for LaAlO3 overlayers on SrTiO3: Domestication of the Polar Catastrophe

Warren E. Pickett

When growing layers of one ionic material on top of another with a differing type of formal charge per layer (LaAlO3 on SrTiO3, say, where layer charges are +1/-1 and 0/0 respectively), there is a local charge mismatch at the interface that has attracted great interest. As one grows such a system and assuming the formal ionic charges persist, an increasingly large electric dipole forms. This is known as the polar catastrophe: the dipole potential grows with limit. This cannot be sustained to very many layers, and the questions is: what happens, when does it happen, and how does it happen? Density functional theory calculations reveal that the strong ferroelectric distortions screen the dipolar electric field (much more strongly than the electronic screening from LaAlO3), and sustain the formal charges (the system remains insulating) up to five unit cells of LaAlO3 on SrTiO3; at this point interesting metallization occurs which requires further calculations to really understand. "Capping" SrTiO3 layers produce surprising changes, which will also be discussed.

** in collaboration with Rossitza Pentcheva.

Imaging submicron ferroelectric domains with slow electrons

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Magnetic multiferroic materials simultaneously display ferroelectric and (anti-)ferromagnetic order. Magnetoelectric coupling, i.e., the cross-linking of magnetization and dielectric polarization makes multiferroics particularly appealing for applications. This phenomenon could be exploited for new concepts of devices such as electric field-controlled magnetic data storage or magnetic field-controlled ferroelectric memories. Currently there are two major technical obstacles to the technical development of single phase multiferroics for spintronic devices: first, only a very small fraction of the existing single-phase multiferroics shows robust electric and magnetic polarization at room temperature; second, the study of the fundamental properties of multiferroic materials requires the use of new analysis techniques and multi-method instruments to study both the electric and the magnetic properties.

Photoemission electron microscopy (PEEM) combined with x-ray linear or circular magnetic dichroism is among the most promising techniques to investigate the magnetic properties, since it provides local spectroscopic information and it can be used for high-resolution imaging of magnetic domains in multiferroics. In addition to the access to the magnetic order, we have recently demonstrated the possibility of imaging ferroelectric domains using low-energy electrons in a combined PEEM-LEEM microscope. The delicate sensitivity of ultra-low energy electrons to small electric surface potential variations has been exploited to resolve periodically “up” and “down”-polarized ferroelectric strips with deep submicron resolution. These low-energy electron microscopy images are compared to piezoelectric force microscopy results to confirm the possibility of imaging ferroelectric domains using slow electrons. The contrast mechanism creation will be explained in this presentation, based on the distribution of the equipotential surfaces calculated using the finite element method.

This high-resolution, direct electron imaging method of ferroelectric domains may open new possibilities for the investigation of domains and domain wall propagation dynamics in multiferroics, in particular when combined with XMC(L)D-PEEM.

Atomic-scale study of electric dipoles near 180° domain walls in ferroelectric films

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Ferroelectrics are materials exhibiting spontaneous electric polarization due to dipoles formed by displacements of charged ions inside the crystal unit cell. Their exceptional properties are exploited in a variety of microelectronic applications. The electronic memory devices function based on the switchable polarization by external electrical field. The polarization switching is realized by the movement of polarization domain walls. The behavior of the dipoles at the domain walls is thus the key issue for understanding the polarization switching and thus the device performance. Using the negative spherical-aberration imaging technique in an aberration-corrected transmission electron microscope we investigate the cation-oxygen dipoles near 180° domain walls in epitaxial $PbZr_{0.2}Ti_{0.8}O_3$ thin films on the atomic scale. The width and dipole distortion across the walls are measured, and on this basis the local polarization is calculated.

Spectroscopy of electronic reconstructions at oxide interfaces

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We will discuss recent experiments using a combination neutron reflectometry, x-ray spectroscopy, and spectral ellipsometry to probe charge transport as well as magnetic and orbital polarization at oxide interfaces. Of particular interest will be cuprate-manganate [1-3] and nickelate [4] interfaces. The latter experiments indicate an intrinsic metal-insulator transition at the interface driven by charge ordering.

[1] J. Chakhalian et al., Nature Phys. 2, 244 (2006)
[2] J. Chakhalian et al., Science 318, 1114 (2007)
[3] J. Freeland et al., Appl. Phys. Lett. 90, 242502 (2007)
[4] A. Boris, Y. Matiks, H.J. Kim, P. Leininger, H.U. Habermeier, G. Cristiani, B. Keimer (unpublished)

Screening mechanism for polar discontinuity for $LaAlO_3/SrTiO_3$ thin films

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We perform a systematic study of electronic structures and potential profiles based on the *ab initio* calculations for $LaAlO_3/SrTiO_3$ (001)-stacking thin films, $(TiO_2\text{-}SrO)_2(AlO_2\text{-}LaO)_n$ and $(SrO\text{-}TiO_2)_2(LaO\text{-}AlO_2)_n$ ($n = 1\sim5$), with and without atomic position relaxation. To eliminate artifacts from periodic boundary condition, the exact Coulomb cutoff technique (Rozzi et al.: Phys. Rev. B **73** 205119 (2006))) is applied.

Without atomic position relaxation, the system is a metal for all the 10 cases. In contrast, with atomic position relaxation, systems with $n \leq 3$ have finite band gaps, while those with $n = 4$ and 5 are metals. However, careful inspection reveals that even for $n = 4$ and 5, the n-type interface ($LaO\text{-}TiO_2$) is conducting while the p-type interface ($SrO\text{-}AlO_2$) is insulating. Screening mechanisms are discussed for cases with and without atomic position relaxation.

Electronic structure induced reconstruction and magnetic ordering at the $LaAlO_3|SrTiO_3$ interface

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Using local density approximation (LDA) calculations we predict $GdFeO_3$-like rotation of TiO_6 octahedra at the n-type interface between $LaAlO_3$ and $SrTiO_3$. The narrowing of the Ti d bandwidth which results means that for very modest values of U, LDA+U calculations predict charge and spin ordering at the interface. Recent experimental evidence for magnetic interface ordering may be understood in terms of the close proximity of an antiferromagnetic insulating ground state to a ferromagnetic metallic excited state.

PACS numbers:

Modeling of Magnetoelectric Interfaces

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Controlling magnetic properties of a ferromagnetic material by electric fields through the magnetoelectric effect has recently attracted significant interest due to new functionalities not available in conventional electronic and magnetic devices. One of the promising ways to achieve a strong magnetoelectric 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 theoretical studies of these magnetoelectric interfaces and ferroelectric tunnel junctions which are interesting for application in multifunctional electronic devices.

Strain-mediated electric effects in ferroic heterostructures and tunnel junctions

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In ferroelectrics and ferromagnets, considerable lattice strains may be induced by an external electric and magnetic field, respectively. These strains are expected to affect many physical characteristics of ferroic material systems. In this talk, the theoretical predictions of two important strain-mediated electric effects in ferroic heterostructures will be discussed.

In the fist part of the talk, the quantum mechanical electron tunneling across ultrathin ferroelectric barriers will be analyzed. Owing to the converse piezoelectric effect inherent in ferroelectric materials, the electric field applied to a ferroelectric tunnel junction (FTJ) creates significant lattice strains in the barrier. These piezoelectric strains modify the barrier thickness, electron effective mass, and position of the conduction-band edge in the barrier. As a result, the current-voltage (*I*-*V*) relationship becomes qualitatively different from the *I*-*V* characteristics of conventional tunnel junctions. Remarkably, the conductance minimum becomes shifted from zero voltage, and a resistive switching takes place after the polarization reversal in a ferroelectric barrier. Hence the *I*-*V* characteristic appears to be hysteretic even in a symmetric FTJ with identical electrodes. In asymmetric junctions with dissimilar electrodes, the resistance on/off ratio is dominated by the depolarizing-field effect associated with imperfect screening of polarization charges at the film/electrode interfaces, but the piezoelectric strains affect the shape of *I*-*V* curve even in strongly asymmetric junctions.

The second part of this talk will be devoted to the theoretical description of a giant magnetoelectric effect which may occur in multiferroic film/substrate systems involving ferromagnetic and ferroelectric constituents. If the substrate is made of a ferroelectric material with a high piezoelectric response, considerable macroscopic strains may be induced in the substrate by an external electric field. Via the interfacial coupling in the film/substrate system, the field-induced substrate deformations change the in-plane lattice strains in a ferromagnetic film, which may affect the magnetization orientation due to the magnetoelastic interaction. The nonlinear thermodynamic theory shows that the resulting magnetoelectric effect becomes especially strong when the misfit strain in the film/substrate system is close to a critical value so that additional deformations induced by the applied electric field lead to the spin-reorientation transition in a ferromagnetic film. The calculations performed for $CoFe_2O_4$ and Ni films grown on crystals of relaxor ferroelectrics demonstrate that the magnetoelectric susceptibility of such ferromagnetic/ferroelectric heterostructures may reach giant values exceeding 10^{-6} s/m.

THE EFFECT OF STRAIN ON THIN FERROELECTRIC AND MULTIFERROIC LAYERS

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Using epitaxy and the misfit strain imposed by an underlying substrate, we have strained ferroelectric and multiferroic thin films to percent levels—far beyond where they would crack in bulk. Under such strains, the ferroelectric properties of $SrTiO_3$, $BaTiO_3$, $EuTiO_3$, and $BaTiO_3/SrTiO_3$ superlattices are dramatically altered. Materials that are not ferroelectric or multiferroic in their unstrained state are made ferroelectric or multiferroic by strain, the transition temperature (T_C) of ferroelectric materials is increased by *hundreds* of degrees, and superlattices containing a strained $BaTiO_3$ layer just one unit cell thick (4 Å thick) remain ferroelectric. Thin $SrTiO_3$ films are made ferroelectric by commensurately straining them to silicon. Our approach to controlling the properties of ferroelectric and multiferroic films centers on the use of substrates (e.g., $ReScO_3$) that enable the growth of uniformly strained films below, or at least far closer to, the critical thickness for relaxation. Our results show that for thin films, which are relevant for tunnel junctions, strain is a viable alternative to the traditional method of chemical substitutions for shifting T_C by large amounts.

Magnetoelastic magnetization manipulation in ferromagnet/ferroelectric hybrids

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The functionality of magnetoelectronic devices hinges on the magnetization orientation. Multifunctional ferromagnetic/ferroelectric hybrids hold the promise for an electric field control of magnetization, enabling the realization of novel, all-electrically controlled magnetoelectronics.

We here discuss the voltage-control of magnetization orientation in ferromagnetic thin film/piezoelectric actuator hybrid structures. To this end, thin ferromagnetic Ni, Fe_3O_4, or $Ga_{1-x}Mn_xAs$ thin films were evaporated or cemented onto commercially available piezoelectric stacks. The application of an electric voltage to the actuator results in an elongation, which is directly transferred into the ferromagnet. Due to magnetoelastic coupling, the voltage-controlled strain significantly modifies the magnetic anisotropy of the ferromagnet and allows to tune the magnetization orientation.

Using ferromagnetic resonance, magneto-optical Kerr effect, and anisotropic magnetoresistance techniques, we have quantitatively determined the magnetic anisotropy and the magnetization orientation within the plane of the ferromagnetic films in our samples. These experiments show that upon the application of a voltage to the piezoelectric actuator, the strain-induced modifications of magnetic anisotropy allow for a continuous and fully reversible control of magnetization orientation within a rotation range of up to 70°. Furthermore, a remanent control of the magnetization orientation also is possible, allowing to realize a simple, all-electrically controlled magnetic memory cell.

Oxide based heterostructures for spintronics

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The role of oxides in electronics has continuously increased over the past few years. The field of spintronics is no exception. This is due to the large diversity of their physical properties and the potentiality to modulate them. In particular, perovskite oxides exhibit an exceptionally broad range of functionalities: they can be insulators, semiconductors, metals, superconductors, heavy fermion systems, ferromagnets, antiferromagnets, ferroelectrics, piezoelectric or even multiferroics [1]. This is even further enlarged by the possibility to obtain new properties at the interface. To illustrate these points, we will present results obtained on multiferroic based heterostructures [2] in which it is possible to either exploit the multifunctional character of the compound or take advantage of the presence of a magnetoelectric coupling between the ferroelectric and antiferromagnetic orders. We will also present recent results on the conduction at the interface between two insulating materials $SrTiO_3$ and $LaAlO_3$ and the experiments we have performed in order to determine the extension of this electron gas [3].

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EuO_{1-x} – A Half-Metallic Ferromagnetic Semiconductor with High Potential for Application Driven Science

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The ferromagnetic semiconductor europium oxide (T_C = 69 K) exhibits a multitude of giant properties such as metal-to-insulator transitions (MIT) that can cover up to 13 orders of magnitude change in resistance, colossal magneto-resistive (CMR) effects that rank amongst the biggest for bulk materials and the largest magneto-optic effects for any known material. Despite these outstanding properties, its instability in air has hampered its utilization for basic and device driven research since its discovery in the 1960's, when the core of today's knowledge about this material was established. Its predicted spin-polarization of 100% in the ferromagnetic state and its excellent electronic compatibility to the long spin decoherence length semiconductor silicon have spawned new interest in EuO in the rapidly growing field of spin-electronics. Here we report about the epitaxial growth of EuO on various substrates including Si and GaN. To prevent the corrosion of the films in air, special capping and patterning techniques have been developed, allowing for the *ex situ* manipulation and measurements of the films as well as for the realization of complex device structures. Using two MBE-based growth techniques, flux matching and adsorption control, we demonstrate the best crystalline quality, the highest magnetization, and the most pronounced MITs and CMR effects reported for EuO films so far. By employing Andreev reflection spectroscopy we show spin-polarizations of lanthanum doped EuO exceeding 90% [1]. With the reported growth and processing techniques, we show a route for further investigations of this outstanding material in basic- and device-driven science as well as its utilization in spinelectronics.

[1] A. Schmehl *et al.*, Nat. Mater. **6**, 882 (2007)

Influence of strain relaxation and interface configuration on the dielectric response of ferroelectric BST thin film capacitors

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The collapse of the dielectric response which is commonly observed in $Ba_xSr_{1-x}TiO_3$ (BST) thin films is a topic of general physical interest as well as a key issue in terms of a possible application of this material in future DRAM storage capacitors. We addressed the influence of substrates-imposed strain and electrode interface configuration on the ferroelectric properties of epitaxial $SrRuO_3$/BST/$SrRuO_3$ thin film capacitors. The growth mode of BST thin films was analyzed by RHEED and HRTEM from the thickness range of a few unit cells up to hundreds of nanometers where plastic strain relaxation occurs. The crystalline quality of our ultrathin samples enabled us to resolve the atomic arrangement and to identify the terminating layers at the $SrRuO_3$-BST interface by HAADF-STEM analysis. We obtained bulk-like permittivities in the order of 5000 and its thickness dependence can be well described by an extended Ginzburg-Landau-Devonshire model by taking into account plastic strain relaxation in BST thin films and finite screening of depolarizing fields by the SRO electrodes. We will furthermore present relaxor-type behavior of the BST thin films that becomes visible only in samples with sufficient interface quality and hints on nanoscale structural inhomogeneities.

Kondo Proximity Effect: How Does a Metal Penetrate Into a Mott Insulator?

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We consider a heterostructure of a metal and a paramagnetic Mott insulator using an adaptation of dynamical mean-field theory to describe inhomogeneous correlated systems [Phys. Rev. Lett. **101**, 066802 (2008)]. The metal can penetrate into the insulator via the Kondo effect. We investigate the scaling properties of the metal-insulator interface close to the critical point of the Mott insulator. At criticality, the quasiparticle weight decays as $1/x^2$ with distance x from the metal within our mean-field theory. Our numerical results (using the numerical renormalization group as an impurity solver) show that the prefactor of this power law is extremely small, implying that the Mott insulator is *de facto* impenetrable to the metal. We discuss extensions of our approach to deal with charge reconstruction at interfaces.

Ferromagnetic correlations at atomically-engineered manganite interfaces

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Abstract

Modifications of electron correlations at perovskite heterointerfaces have recently received much attention. This is partly due to advances in growth control at the atomic scale, and also due to advances in characterization techniques that are able to distinguish properties of the interface region from those of the bulk. This talk will focus on modifications to the complex double-exchange-mediated ferromagnetism in manganites that occur near a manganite-insulator interface that has been atomically "designed". The underlying mechanisms for weakened ferromagnetic correlations at manganite interfaces might be understood by systematically quantifying the magnetization profiles of interfaces grown with different atomic stacking sequences, doping profiles and lattice strain. I will present our work on improving both the growth and characterization aspects of this problem. First, I will outline our approach to improve control of atomic layering during interface growth in our home-built oxide MBE system, combining different layering methods and careful RHEED rocking curve analysis. Second, I will discuss our characterization of interfacial magnetization profiles, and their evolution in temperature, by X-ray resonant magnetic scattering (XRMS) using synchrotron radiation tuned to the manganese L2,3 absorption edge, and future experiments with lateral resolution using photoemission electron microscopy (PEEM). The goal is to determine if suitable design of the interface can reinforce double-exchange correlations at higher temperatures in the last manganite layer, and mitigate the effects of nanoscale phase separation. While this talk focuses on magnetism at manganite/insulator interfaces, we hope that this approach of interface engineering and characterization could be more generally applied to study, and perhaps tune, electron correlations in different transition-metal oxide interfaces in the future.

Probing ferroelectricity in ultrathin wedged epitaxial $BaTiO_3$ films

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High quality epitaxial wedged $BaTiO_3$ ultrathin films were grown epitaxially on $SrRuO_3$-covered (001) - oriented $SrTiO_3$ substrates by high-pressure sputtering.
The crystallinity, the composition and the surface roughness along the wedged $BaTiO_3$ films were verified by x-ray diffraction, Rutherford Backscattering Spectrometry (RBS) and atomic force microscopy, respectively.
The thickness profile along the wedge film and the in-plane and out-of plane lattice parameters of the wedge were studied by x-ray diffraction using a laboratory source and synchrotron radiation. The $BaTiO_3$ films were fully strained by the substrate.
Ferroelectric capacitors were then fabricated from $SrTiO_3/SrRuO_3/BaTiO_3$(wedge)$/SrRuO_3$/Pt hetero-structures using optical lithography and ion beam etching. Electrical hystersis loop measurements along wedge of 3.5 nm to 5.4 nm showed a reduction of the polarization from 43 $\mu C/cm^2$ to 26 $\mu C/cm^2$.
Leakage current was compensated by subtracting a quasi-static I-V leakage curve from the I-V curve obtained at 30 kHz.
In general wedge oxide films are an interesting approach to extract in a time saving manner important characteristic parameters in a single run with small spread, and they are suitable for size effects studies.

Magnetic phase transition in two-phase multiferroics predicted from first principles

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On the basis of first-principles electronic-structure calculations we predict that epitaxial multiferroic films—fabricated as ultrathin Fe films deposited on TiO_2-terminated (001) surfaces of $ATiO_3$ perovskites (A = Pb, Ba)—exhibit an unexpected change of their magnetic structure with increasing Fe-film thickness. The magnetic order changes from ferromagnetic, with a magnetization of about $3\,\mu_{\mathrm{B}}/\mathrm{atom}$ for the 1-monolayer system, to ferrimagnetic with almost vanishing magnetization upon deposition of a second Fe layer. Ferromagnetic order is restored for thicker Fe films but with significantly reduced magnetization as compared to Fe bulk. The effect is understood in terms of hybridization of electronic states and geometric structure. The magnetoelectric coupling affects the size of the magnetic moments moderately, a spin-reorientation transition is not found.

All-Electron GW Calculations for Strontium and Barium Titanate

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The GW approximation for the electronic self-energy yields quasiparticle band structures in very good agreement with experiment, but almost all implementations so far are based on the pseudopotential approach, which limits their range of applicability. We have developed an implementation (SPEX, http://www.flapw.de/spex/) within the full-potential linearized augmented-plane-wave (FLAPW) method, which treats core and valence electrons on an equal footing. Within this method a large variety of materials can be treated, including d- and f-electron systems, oxides and magnetic systems. We discuss results for two prototype $\mathrm{ABO_3}$ semiconductors, paraelectric $\mathrm{SrTiO_3}$ and ferroelectric $\mathrm{BaTiO_3}$, which are widely used in electronic applications. Their band gaps are difficult to measure experimentally and have been under debate for a long time. Ab initio theoretical studies of their electronic structure have mostly been based on density-functional theory so far, which showed a strong underestimation of the band gaps. Here we present GW calculations that overcome this problem and yield band gaps very close to the best experimental estimates. Financial support from the Deutsche Forschungsgemeinschaft through the Priority Programme 1145 is gratefully acknowledged.

Magnetic tunnel junctions with ferroelectric tunnel barriers : electroresistance and tunneling magnetoresistance

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Ferroelectric thin films are a subject of great interest for applications in electronic devices such as FeRAMs[1]. Ferroelectric thin films have been extensively studied within the last few years and leakage currents are one of the factors limiting the performance of these capacitive devices. When the thickness of the films reaches a few nanometers, the main leakage mechanism is tunneling (direct or Fowler-Nordheim)[2]. In this regime, the leakage current is predicted to depend critically on the polarization direction. It seems possible to wisely make the most of the leakage current, so detrimental for state-of-the-art FeRAMs, to read the information stored by the electrical polarization and define a new type of non capacitive ferroelectric memories in which the main advantage is non-destructive read-out. In principle, such ferroelectric tunnel junctions (FTJ)[2], thus exhibit a hysteretic tunneling electroresistance effect (TER) associated with the hysteretic dependence of the polarization on the bias voltage. In fact, FTSs share similarities with magnetic tunnel junctions that are made of ferromagnetic electrodes sandwiching a thin dielectric layer. The relative change of the magnetizations of the electrodes (parallel / antiparallel) leads to two distinct resistance states and a consecutive tunneling magnetoresistance effect (TMR). Replacing widely used non polar dielectric barriers by ferroelectrics could give rise to combined TER and TMR effects[3]. A critical issue is then the persistence of ferroelectricity at film thicknesses compatible with direct tunneling (a few unit-cells)[4]. Pioneering investigations of Gajek *et al.* with multiferroic (ferroelectric and ferromagnetic) tunnel barriers of $La_{0.1}Bi_{0.9}MnO_3$ demonstrated these two effects in a device with four distinct resistance states[5]. In order to optimize independently these two effects and understand better the underlying mechanisms, it is more attractive to isolate the origin of the tunnel electroresistance (in the ferroelectric barrier) from the origin of the tunnel magnetoresistance (in the ferromagnetic electrodes).

To address this issue we have investigated magnetic tunnel junctions with ferroelectric tunnel barriers of $BaTiO_3$ (BTO). Growth conditions were optimized to obtain epitaxial thin films of BTO over thin ferromagnetic films of $La_{2/3}Sr_{1/3}MnO_3$ (LSMO). The ferroelectric character of 30 nm BTO thin films has been demonstrated by piezoforce microscopy (PFM). Through resistivity measurements on ultrathin films of BTO (1.5-5 nm), we validated tunneling as the main transport mechanism. Nanojunctions of LSMO/BTO/(Co, Au) were defined by a technique developed at CNRS/Thales[6]. We observed tunnel magnetoresistance effects (TMR) of 13% at low temperature in LSMO/BTO/Co junctions, indicative of spin-dependent tunneling through BTO. In addition, applying large voltage pulses in LSMO/BTO/Au junctions lead to clear and reproducible changes of the tunnel resistance (TER) of around 100%. We will discuss the possible origin of this TER considering several mechanisms, including the ferroelectric character of the 2.5 nm BTO layer. Finally we will show that combining BTO tunnel barriers with different ferromagnetic electrodes can give rise to modifications of TMR effects upon switching the electric polarization of BTO.

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Noncollinear Magnetism in the Perovskite Manganite Superlattice

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Recently, artificial superlattice composed of different magnetic structures attract much attention as candidates for spintronics materials such as tunnel magnetoresistance device[1]. Perovskite manganites $La_{1-x}Sr_xMnO_3$ (LSMO) is very hopeful material as a spintronics device, because LSMO shows the colossal magnetoresistance and half-metallic properties[2]. It was reported that the magnetic frustration due to different magnetic phases induces the noncollinear magnetism at a superlattice interface[3]. In order to enhance the potential as a spintronics device, it is important to analyze the magnetic structure of interface on the basis of electronic states.

In the present work, we have performed noncollinear density-functional calculations on perovskite manganites bulk LSMO and superlattice $(LaMnO_3)_m/(SrMnO_3)_n$. We found that the noncollinear magnetic state is stable by carrier doping in the bulk and superlattice interface. We will discuss the correlation between the stability of noncollinear magnetic states and lattice distortions.

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A novel total electron yield set-up for interface studies under soft x-ray radiation and a simultaneously applied bias field

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We used soft x-ray absorption spectroscopy of the total electron yield (TEY) mode to study the ferroelectric capacitors under a simultaneously applied bias. Pt/$PbZr_{0.3}Ti_{0.7}O_3$(PZT)/Pt ferroelectric capacitors were deposited on platinized Si/SiO_2 substrates. The PZT was (111) oriented. Seven capacitors with an area of A=3.425 mm^2 each were fabricated by optical lithography and Ar ion milling. The etching was stopped after reaching the PZT layer by using a mass spectrometer. The coercive fields +/- E_c were determined to +110 kV/cm (V_{c+}= 2V) and –67 kV/cm (V_{c-}= -1.2V). The samples were placed in the undulator beam line 8 at the Advanced Light Source. The leads of both, top and bottom electrodes, were connected to an external circuitry including two ammeters and a voltage source. This TEY set-up allowed us to investigate the Titanium $L_{2,3}$-edge and Oxygen absorption *K*-edge of the ferroelectric insulator adjacent to the Pt electrodes in dependency of the external applied potential or the negative or positive remnant polarization state of the ferroelectric capacitors. The current distribution under soft-x-rays is discussed in the framework of the inner and external photoelectric effect. Modifications of the crystal field splitting Δ_{CF}, at the Titanium *L*-edge were observed in dependency of the polarization state of the ferroelectric capacitor. At the Oxygen *K*-edge we observed strongly distorted absorption signals in dependency of the electrical boundary conditions of the capacitors. This might indicate a photo catalytic effect. Hereby the oxygen is redistributed due to the internal electric field and simultaneous soft x-ray radiation. The experimental results are of importance for the understanding of insulator/metal interfaces under an externally applied field and demonstrate such an approach might be in general useful for various ferroelectric devices as well as for oxide/metal interfaces

Non-equilibrium surface and bulk spin-dynamics at Gd(0001)

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In solids the charge, lattice, and spin degrees of freedom are coupled and respective coupling strengths result in characteristic timescales on which excitations of one particular subsystem interact and equilibrate with the remaining subsystems. In ferromagnetic metals the respective elementary interaction processes occur on the pico- and femtosecond time scale. To elucidate these interaction mechanisms and the timescales we investigate the ultrafast spin dynamics excited by intense infrared optical pulse at the Gd(0001) surface and in the bulk of Gd, employing such complementary time-resolved methods as: (i) the magnetic linear dichroism of the Gd 4f core-level in a photoemission at Gd(0001) measured at BESSY employing 1.55eV, 100fs laser pump and 60eV, 50ps synchrotron-radiation probe-pulses [1]; (ii) X-ray magnetic circular dichroism experiments at Gd $M_{4,5}$ absorption edges measured at the fs-slicing facility at BESSY using polycrystalline Gd films; (iii) MOKE investigated at Gd(0001) using 1.55eV, 35fs laser pump and probe pulses with simultaneous detection of (iv) second harmonic generation. The last method is sensitive to the transient surface magnetization M_S while techniques (i)-(iii) monitor the transient bulk magnetization M_B. From the similarity of the results of methods (i)-(iii), we conclude that MOKE also monitors the dynamics of 4f spins (or the spin dynamics of valence electrons is identical to that of 4f electrons). M_B decreases in 2 steps at 1ps and 50ps time scales due to interaction of 4f spins with hot electrons and lattice, respectively. The reduction of M_S occurs on the ultrafast time scale only, and 1ps decrease induced by hot electrons is preceded by much stronger break-down during the direct laser excitation. It is coursed by an effective spin-flip during the re-screening of photo-holes in the surface layer [2] leading to a 5 times larger ultrafast decrease of M_S in comparison to that of M_B. The equilibration of M_S and M_B takes ~200-500 ps, which is contra-intuitive but can be explained by fast (on a scale of 1ps) expansion of the distance between surface and next-to-surface atomic planes coursed by the surface spin-flip [2]. With that the system is trapped in a meta-stable state. The related elementary processes will be discussed.

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Tunneling across a ferroelectric barrier : a first-principles study

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Ferroelectric tunnel junctions (FTJ), including a ferroelectric as the barrier material, have recently attracted a lot of interest since they are potentially interesting for technological applications such as data storage. In such system, the barrier has to be sufficiently thin to allow for tunneling but must at the same time remain ferroelectric, a property that tends to be suppressed in ultrathin films. Up to now, the modeling of FTJ has remained at the semi-empirical level. Here, we consider a prototypical system made of a ferroelectric oxide film between two gold electrodes and compute the I-V curve of the system using density functional theory and Non-Equilibrium Green's Function (NEGF+DFT) formalism. Our atomic-scale approach allows for the first time accurate and self-consistent description of the screening at the metal ferroelectric interface and of the atomic relaxation. It predicts that the asymmetry in the I-V curve for up and down polarizations is sufficiently large to be detected experimentally, therefore opening the door to applications in which the tunneling current allows the reading of the polarization state. Work supported by FAME-EMMI.

First-principles investigation of thin ATiO$_3$ films with stacking faults

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Experimental studies have shown that defects and stacking faults play an important role in ferroelectric materials. Employing density functional theory calculations based on the full-potential linearized augmented planewave (FLAPW) method as implemented in the FLEUR code (www.flapw.de), we study the polarization of thin films of the perovskite ATiO$_3$ compounds PbTiO$_3$ and BaTiO$_3$. Both AO-terminated and TiO$_2$-terminated surfaces with the polarization in the film plane and perpendicular to the surface are considered. We present studies on the applicability of different exchange-correlation potentials and present results on the influence of stacking faults and defects at the surfaces on the ferroelectric polarization in these compounds. While the impact of these structural imperfections on an in-plane oriented polarization is short ranged, they have far-reaching consequences for a ferroelectric polarization perpendicular to the surface.

Microscopic origin of magnetism in hematite - ilmenite heterostructures

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Charge mismatch at complex oxide interfaces can give rise to properties and functionality entirely different from the parent compounds. For example nanoscale lamellar exsolutions between the canted antiferromagnet haematite and the room temperature (RT) paramagnet ilmenite show unique magnetic properties. To explain the origin of magnetism in the Fe_2O_3-$FeTiO_3$ system we have performed density functional theory calculations systematically varying the concentration, distribution and charge state of Ti (Fe) incorporated in a α-Fe_2O_3 ($FeTiO_3$) host. We use the all-electron full-potential linearized augmented plane wave method in the WIEN2k implementation. Our investigation shows that including electronic correlation within the LDA+U approach is decisive to obtain the correct magnetic ground state and band gap of the end members, $Fe^{3+}{}_2O_3$ and $Fe^{2+}Ti^{4+}O_3$.

The phase diagram of the stability with respect to the end members for more than 30 different configurations reveals a clear preference to form layered arrangements as opposed to solid solutions. We find that the charge mismatch at the interface between Fe_2O_3 and $FeTiO_3$ is accommodated through Ti^{4+} and a disproportionation in the Fe contact layer into Fe^{2+}, Fe^{3+}. This leads to uncompensated moments in the contact layer and gives first theoretical evidence for the lamellar magnetism hypothesis [1]. This interface magnetism is associated with impurity levels in the band gap showing half-metallic behaviour [2] and making Fe_2O_3/$FeTiO_3$ heterostructures prospective materials for spintronics applications.

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XAS and XMCD spectroscopy on $Nd_1Ba_2Cu_3O_7$ /STO interface

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We will present some latest results on the application of the X-ray absorption Spectroscopy and X-ray magnetic circular Dichroism to the study of the electronic properties of metal transition oxides interface of interest for application: $Nd_1Ba_2Cu_3O_7/SrTiO_3$ interface under application of electric field. We will show that the mechanism of the electric field effect doping is similar to the chemical doping, i.e. occurs by charge transfer of carriers from the heavily doped charge reservoir, composed by chains, to the Zhang-Rice band of the CuO_2 planes

Correlation between stacking defect and resistive switching in Sr_2TiO_4 thin films

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A great deal of effort on reversible resistive switching has been done in oxide materials. However, the precise mechanisms are still unclear. One of the reasons is due to relatively high defect density in oxides. Unfortunately it is not easy to exclude the influence of lattice defects, even in a high quality single crystal [1]. On the contrary, lattice defect has a potential to work as charge traps, conduction filaments, and/or easy diffusion ion paths. In the sense, it is useful for understanding the mechanism to investigate resistive switching properties under control of lattice defects in channel. In this study, we present the crystal growth and resistive switching properties of Sr_2TiO_4 thin films with the aim of defect engineering.

Non-doped Sr_2TiO_4 films were epitaxially grown on $SrTiO_3$ (001) substrates by pulsed laser deposition (PLD). Laser energy density, substrate temperature, and oxygen pressure during deposition were carefully adjusted to obtain stoichiometric films. At a low growth temperature of 700 C, random distribution of SrO double layers both laterally and vertically was observed in TEM images. This resulted in the disappearance of some peaks in XRD because a new extinction rule was created by the random distribution. On the other hand, films grown at a higher temperature of 900 C showed well-ordered structure due to large thermal energy which compensates local nanometer-scale nonstoichiometry of deposited adatoms [2]. For electrical measurements, Nb-doped $SrTiO_3$ substrates were used as a bottom electrode. Gold top electrodes were evaporated. Films grown at the low temperature that include high-density defects showed clear switching properties with a high on/off resistance ratio after an electrical forming process. In contrast, poor switching hysteresis was seen in well-ordered films. This clearly demonstrated the correlation between stacking defect and resistive switching in Sr_2TiO_4 thin films.

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Theoretical study of $La_{1-x}Sr_xMnO_3/BiFeO_3$ heterojunction: Exchange bias and magnetoelectric coupling

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The exchange bias effect [1], which induces a unidirectional shift of the magnetic hysteresis loop at ferromagnetic/antiferromagnetic interface, is important to control the nano-scale magnetic property for the spintronic applications. Recently, in order to develop the multifunctionality in a device, ferromagnetic/antiferromagnetic-ferroelectric heterostructure is considered as a candidate for the multiferroic exchange bias interface [2]. In this context, we have theoretically investigated the exchange bias and the magnetoelectric effect in $La_{1-x}Sr_xMnO_3$ (LSMO) / $BiFeO_3$ (BFO) heterojunction. First, we have performed *ab-initio* density functional calculations of the magnetic property in the optimized [001]-oriented LSMO/BFO heterostructure by using VASP program code. Using the calculated total energy and the Heisenberg Hamiltonian, the superexchange interaction energy J_{ij} between Mn and Fe spins at the interface was estimated. Second, using the calculated value of J_{ij}, we have performed a Monte Carlo simulation to obtain the hysteresis loop by flipping the Mn spins with applied magnetic field. The result shows that the exchange bias shift is induced by the existence of magnetic domains at the antiferromagnetic BFO layers, which is stabilized by the intermixing of the Mn and Fe sites at the interface layer. The finding is well consistent with the earlier model of Malozemoff [3]. In this session, we will focus on the discussion on the nature of the exchange bias effect in the LSMO/BFO interface and how it is affected by the magnetic coupling and the structural roughness at the interface layer, and in addition, by the ferroelectricity in BFO layers.

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$(Sr,Mn)TiO_3$ - a magnetoelectric multiglass

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By analogy with the well-known multiferroic materials a 'multiglass' scenario is encountered, if two different glassy states are found simultaneously in one and the same solid system. Such a situation has been found in the oxide system $(Sr_{0.98}Mn_{0.02})TiO_3$, where Mn^{2+} ions randomly occupy Sr^{2+} lattice sites. Enabled by their small ionic size they go off-center, form interacting electric dipoles, and undergo a dipole glass transition at $T_g(e) = 38$ K. Subsequently, the Mn^{2+} spins ($S = 5/2$) freeze independently into a spin glass at $T_g(m) = 34$ K [1]. Both systems meet crucial criteria of generic glass behavior (divergent relaxation times at T_g, memory and rejuvenation after aging etc.). In addition they show strong magnetoelectric coupling supported by large optical soft-mode fluctuations in the host crystal, $SrTiO_3$, which comes close to a ferroelectric lattice instability. Its high order (E^2H^2) makes on principle the only difference between multiferroic and multiglass systems, where 'electric frustration goes for magnetic freezing'. In addition, sizeable EH^2 coupling has been observed. The required long-range electric ordering is explained by self-poling of the nearly ferroelectric host material.

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Double perovskite multiferroics: the room temperature challenge
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Multiferroic materials are currently one of the spots of high interest in spintronics investigations. Reasons for this are numerous possible applications such as 8-bit memory and possibility of electric field controlled magnetization or magnetic field controlled electric polarization.
We investigate multiferroic double perovskite compounds ($A_2BB'O_6$) focusing on one of the main challenges for the applications of multiferroics: ferroelecticity accompanied by a net magnetization at room temperature. Combining a 3*d* and a 5*d* element at the B and B' sites in an ordered fashion leads to the increase of the magnetic ordering temperature of these ferrimagnets. We demonstrate the role of the "lone pair" of electrons on the A-site atom in inducing ferroelectricity, as well as the possibility of strain-assisted switching between antiferroelectric and ferroelectric states.

Electronic structure and effective masses in strained Silicon

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Abstract

Metal-oxide-semiconductors field effect transistors (MOSFETS) based on strained Si become among the most prominent device for modern microelectronics due to their high mobility achievement compared to those based on unstrained Si. As first step of our investigation of strained Si, we have performed electronic band structure calculations of strained Si within the local density approximation of density functional theory including GW many-body corrections. Band structure, deformation potentials and effective masses are obtained for tetragonal (strain along [001] direction), orthorhombic (strain along [110]) and trigonal (strain along [111] direction) distortions of the unit cell. Both tetragonal and orthorhombic distortions of the unit cell induce a valley splittings and warping on the conduction band while a spliting of the light and heavy hole bands is observed at the top of the valence band. These spliting and warping of the bands and valleys will affect considerably the mobility either for holes or electrons in pMOSFET or nMOSFET respectively and will have an important impact on the design of high-performance semiconductor devices.

Ab initio many-body calculation of magnetic excitations in 3d transition metals

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To study excitation spectra of magnetic materials from first principles we have developed a computational scheme based on many-body perturbation theory.
The main quantity of interest is the dynamical transverse spin susceptibility, from which magnetic excitations, including single-particle spin-flip Stoner excitations and collective spin-wave modes as well as their lifetimes, can be obtained. In order to describe spin waves we include appropriate vertex corrections in the form of a multiple-scattering T-matrix, which describes the coupling of electrons and holes with different spin. To reduce the numerical cost for the calculation of the four-point T-matrix we exploit a transformation to maximally localized Wannier functions that takes advantage of the short spatial range of electronic correlation in the partially filled *d* or *f* orbitals of magnetic materials. Our implementation is based on the full-potential linearized augmented plane-wave (FLAPW) method. As an illustration, we show spin-wave spectra and dispersions for the elementary ferromagnets Fe, Co and Ni calculated with our scheme. The results are in good agreement with available experimental data.

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