

**0.0.1 Report on Workshop “European School on
Multiferroics” (ESMF2010)**

L’Aquila, Italy

September 26th - October 1st 2010

Sponsors

Psi-k, ESF through Intelbiomat Network

Organizers

Silvia Picozzi, School director (*CNR-SPIN, IT*)

Manuel Bibes (*CNRS-Thales, FR*)

Jeroen van den Brink (*IFW Dresden, DE*)

Laurent Chapon (*ISIS, UK*)

<http://www.casti.aquila.infn.it/homepages/bismuth/ESMF2010/index.html>

The main goal of the school was to present a comprehensive overview in the exciting and fastly developing field of multiferroics (materials that combine spontaneous long-ranged magnetic and dipolar orders). ESMF2010 gathered 86 participants, in particular 68 students (mainly Europeans, but also including few participants from USA, Japan, South-Africa, etc) and 18 speakers (again, mostly Europeans with three coming from USA). The number of students was as large as previous editions (compared to same cases, even higher), showing that multiferroics continue to attract enormous interests all over the international scientific community. All the lessons were prepared in a way adequate to PhD students, most of the lectures showing first an introductory part with basic concepts and then moving to recent scientific results, in order to give to young participants a flavor of current research activities. In this respect, the lessons were interesting both for people new to the field as well as for participants with longstanding experience in the area. All the speakers were extremely qualified: plenty of examples were given, so as to make the general concepts clear to everybody when applied to specific materials, cases, mechanisms, etc. The schedule implied 4 lessons per day (90 minutes each + 15 minutes of discussions), excluding Wednesday (due to social excursion and dinner) and Friday (closing day) when two lectures only were held. A poster session, including a prize for the best poster presentation, was held on Tuesday September 28th. The organization of the school schedule was largely appreciated by most of the students.

The choice of the location of the ESMF school in 2010 had a somewhat special meaning, since LAquila was struck by a tremendous quake in April 2009 causing 300 casualties and about 60.000 evacuees. After 18 months, the situation

was still rather severe in LAquila (for example, all the historical center, denoted as red zone, was not accessible to people and nobody was and is - allowed to live there or even enter there). Despite many logistic problems that the local-organizer/director had to solve before the event, the school was held at the Faculty of Mathematical, Physical and Natural Sciences of the University of LAquila, with its building located in the peripheral area of LAquila. Being newer and recently constructed, in general less damages were caused by the quake in this area, so that the lesson room as well as the entire building was accessible and available. Moreover, several hotels could be found nearby and a shuttle-bus service connecting the hotels and the university was arranged for the participants.

After two introductory lectures on ferroelectrics (J. M. Triscone) and magnetic oxides (M. J. Coey) in the first day of the school, the talks were addressed into multiferroics and magnetoelectric materials/phenomena and specifically focused on:

- the (co)-existence and cross-coupling between different long-range orders (magnetic, dipolar, ferroelastic, toroidal);
- the search for new materials showing strong magneto-electric coupling and multiferroicity, including handles [such as strain-engineering (K. Dörr) or materials design (C. Ederer)] to tune the relevant properties;
- the novel physical mechanisms at the basis of complex magnetic phase diagrams (S. W. Cheong), encompassing ferroelectricity (statically) induced by magnetic or charge order as well as dynamical magnetoelectric effects (including electromagnons and domain wall dynamics);
- advanced experimental techniques [neutrons (V. Simonet), X-ray magnetic scattering (A. Bombardi), piezo-force microscopy (S. Fusil), high-resolution transmission electron microscopy (M. Varela), etc] particularly suited for the analysis of multiferroics and magnetoelectrics
- examples of theoretical modelling of “electronic” multiferroics, with examples mainly of charge-ordered materials (J. van den Brink and D. Khomskii)
- the importance of symmetry analysis (L. Chapon) and Landau theory in this field, complemented by practical examples of well-known multiferroics
- perspectives for multifunctional applications (J. Fontcuberta, M. Bibes), including electrically controllable spintronic devices or tunnel electro-magnetic junctions

Systems of interest have ranged from bulk compounds [manganites (in their hexagonal and orthorhombic phases, under equilibrium or strained), nickelates, cobaltates, BiFeO₃, EuTiO₃, etc] to composites, from (strained) thin films to (hybrid) nanostructures (I. Mertig). A lesson given by Joel E. Moore on Topological insulators (TI, a topic currently attracting lots of interest), was included

in the program, in particular focused on the connection between TI and orbital magnetoelectric responses.

The students actively participated in the lessons, with lively discussions lasting for all the allocated time (15 minutes for each lesson). They had also the opportunity, during the poster session, to present their own research activity; in particular, one award for the “best poster presentation of ESMF2010” was given to Pauline Rovillain, Univ. Paris 7, for her work on “Electric field effects on spin-modes in BiFeO₃ crystals”.

Finally, we remark that a school website was created and continuously updated (in particular to upload all the presentations given by the speakers so that they could be publicly downloaded):

<http://www.casti.aquila.infn.it/homepages/bismuth/ESMF2010/index.html>

Programme:

Sunday Sept. 26th

18:00-19:30: Welcome Party

19:30: **Prof. Gianluca Ferrini**, *Univ. L'Aquila, Geology Dept.*, "L' Aquila earthquake on April 6th 2009"

Monday Sept. 27th

9:00-9:30: **Silvia Picozzi**, **Ruggero Vaglio**, *CNR-SPIN (IT)*, "Opening"

9:30-11:15: **Jean Marc Triscone**, *University of Geneva (CH)*, "Ferroelectric materials: an introduction to the field and some examples of recent developments"

11:45-13:39: **Michael Coey**, *Trinity College Dublin (IE)*, "Magnetic Oxides; Introduction and New Directions"

15:00-16:45: **Claude Ederer**, *Trinity College Dublin (IE)*, "First principles studies of multiferroic materials"

17:15-19:00: **Joel Moore**, *Dept. of Physics, Univ. of California, Berkeley (US)*, "Topological insulators and orbital magnetoelectric coupling"

Tuesday Sept. 28th

9:00-10:45: **Katrin Dörr**, *IFW-Leibniz Institut Dresden (DE)*, "Strain effects in ferroic oxide films"

11:15-13:00: **Jeroen Van den Brink**, *IFW, Leibniz Institute for Solid State and Materials Research (DE)*, "Multiferroics: Hamiltonian modeling"

13:00-15:00: Poster session

15:00-16:45: **Alessandro Bombardi**, *Diamond Light Source Ltd, Rutherford Appleton Lab (UK)*, "An introduction to x-ray non-resonant and resonant scattering applied to multiferroics"

17:15-19:00: **Virginie Simonet**, *Institut Nel CNRS Grnoble (FR)*, "Neutron scattering a probe for multiferroics and magnetoelectrics"

Wednesday Sept. 29th

9:00-10:45: **Maria Varela**, *Oak Ridge National Lab, TN (USA)*, "An atomic resolution view at complex oxides: progress challenges and applications"

11:15-13:00: **Stéphane Fusil**, *Unit Mixte de Physique CNRS-Thales (FR)*, "BiFeO₃ or the Guinea pig of multiferroics under the magnifier of piezoresponse force microscopy"

15:00-23:00: Social excursion + dinner

Thursday Sept. 30th

9:00-10:45: **Manuel Bibes**, *Unit Mixte de Physique CNRS-Thales (FR)*, "Ferroic and multiferroic tunnel junctions"

11:15-13:00: **Sang-Wook Cheong**, *Rutgers University, NJ (USA)*, “Multiferroic Vortices”

14:30-16:15: **Ingrid Mertig**, *MPI fr Mikrostrukturphysik Halle and Martin-Luther-Universitt Halle-Wittenberg (DE)*, “Magnetoelectric coupling at multiferroic interfaces”

16:45-18:30: **Laurent Chapon**, *ISIS, Rutherford Appleton Lab (UK)*, “Symmetry applied to magnetoelectrics and multiferroics”

Friday Oct. 1st

9:00-10:45: **Daniel Khomskii**, *Univ. Koeln (DE)*, “Multiferroics and beyond”

11:15-13:00: **Josep Fontcuberta**, *Institut de Ciencia de Materials (ICMAB) - CSIC, Barcelona (ES)*, “Electric and magnetic control of magnetization and polarization in multiferroic heterostructures and devices”

13:00-13:15: Closing

List of poster abstracts:

PS1: Electrophoretic Deposition CoFe₂O₄ Nanograins Dispersed in a BaTiO₃ Matrix

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Nanostructured materials presenting a coupling between the electric and magnetic degrees of freedom have been attracting much scientific and technological interest. By combining a piezoelectric ceramic and a magnetostrictive material the elastic interactions between the phases provide the coupling mechanism inducing a magnetoelectric behavior. Recently, the electrophoretic deposition technique (EPD) has been employed for the production of functional thin films due to its versatility for application with different materials and the ability to be scaled-up to large volumes and sizes. In this technique an electric field is applied on a suspension of charged particles that migrate and are deposited on an electrode. Due to this, very small, nanoscopic, particles (with sizes ≤ 30 nm) can be deposited by electrophoresis. Here, composites of electrophoretic deposited cobalt ferrite (CoFe₂O₄-magnetostrictive) nanograins dispersed in a laser ablated barium titanate (BaTiO₃-piezoelectric) matrix were prepared and their structure was studied by X-ray diffraction (XRD) and Raman spectroscopy. Initially, the CoFe₂O₄ nanograins were deposited by electrophoresis on SiPt substrates, becoming dispersed on the substrate surface. They were then heat-treated and subsequently covered by a laser ablation deposited BaTiO₃ thin film, prepared at 600C. The XRD results show that the films were polycrystalline and composed by tetragonal-barium titanate and CoFe₂O₄ with the cubic spinel structure. The Raman spectra presented modes characteristic of the tetragonal-BaTiO₃ structure, along with the ones from the cobalt-ferrite. The barium titanate and cobalt ferrite lattice parameters were calculated from the XRD peak positions and compared with their bulk counterparts. The obtained values indicate that the cobalt ferrite phase was under compressive stress while the barium titanate was under an expansion strain. The influence of the preparation conditions on the structural and dielectric properties of the deposited thin films will be presented.

PS2: Strain effects on ferroelectric polarization in orthorhombic HoMnO₃

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Aiming at increasing the ferroelectric polarization in AFM-E orthorhombic HoMnO₃, we theoretically investigate the in-plane strain effect on the polariza-

tion by means of DFT calculations and model Hamiltonian approaches. Our results show that the net polarization is enhanced under compressive strain, mainly due to an increase of the electronic contribution to polarization, whereas the ionic contribution decreases. We identify the electron-lattice coupling, due to Jahn-Teller (JT) distortion, and its response to strain as the main responsible for the observed behaviour. The JT- induced orbital ordering of occupied Mn-eg electrons in alternating $3x^2-r^2/3y^2-r^2$ orbital states at equilibrium changes to x^2-z^2/y^2-z^2 states under in-plane compressive strain. The asymmetric charge transfer of eg electrons between Mn ions along zig-zag spin chains (typical of the AFM-E spin configuration) is therefore enhanced, possibly explaining the large value of polarization. We reproduce the change of orbital ordering pattern in a degenerate double-exchange model supplemented with electron-phonon interaction. In this picture, the orbital ordering change is related to a change of the Berry phase of eg electrons, which in turn causes an increase of polarization whose origin is purely electronic.

PS3: Influence of Electric Fields on EuO Thin Films

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Ferromagnetic EuO arouses a lot of interest due to a multitude of extreme properties, such as an insulator-metal transition at the Curie temperature, colossal magnetoresistance, and nearly 100% spin polarization of the conduction electrons in the ordered phase. In addition, ferroelectric behaviour was recently predicted for EuO under tensile strain ϵ 4.2%. We propose to overcome this threshold in epitaxial, strained films (here we achieve a strain of \sim 2%) in combination with an externally applied electric field. The 15 nm thick (001) films are grown on YAlO₃ (110) substrate by molecular-beam epitaxy. An amorphous silicon cap layer of 10 nm prevents degradation in air, while a pattern of titanium contacts evaporated onto the surface allows us to apply a voltage parallel to the sample surface. For investigating the electric and magnetic order of the films, we use polarisation dependent optical second harmonic generation (SHG): Due to the inversion symmetric crystal structure, only the latter contributes and can therefore be observed background free. Here, we show the dependence of the SHG intensity on externally applied electric fields in different geometries. Furthermore, the influence on the ferromagnetic transition temperature and on the sample magnetisation is investigated.

PS4: First Principles Modeling Of Spin Transport In Multiferroic Tunnel Junctions

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Spin-dependent tunneling between ferromagnetic electrodes separated by insulating oxide barriers has long attracted scientific and commercial interest. One can ask how the transport properties of such a tunneling junction can be changed and engineered by using functional barriers. The combination of materials with different ferroic states has the prospect of enabling one to actively manipulate the tunneling current with both external magnetic and electric fields [1]. We demonstrate massive tunneling magnetoresistance (TMR) and electroresistance (TER) in junctions made by using functional barriers and both simple metals and oxide electrodes. Ground state electronic structure calculations are performed with density functional theory (DFT) as implemented in the SIESTA package. We use both the conventional local spin-density approximation (LSDA) to band theory as well as an atomic self-interaction correction scheme (ASIC), which allows for a better description of the electronic properties of the ferroelectric material. We furthermore present calculations of the I-V characteristics of these junctions obtained with the electronic transport code Smeagol [2]. The calculations are carried out for different magnetic configurations of the electrodes and ferroelectric configurations of the insulating barrier and demonstrate the intricate interplay between these order parameters.

References

- [1] V. Garcia et al., Nature 460, 81 (2009), P. Maksymovych et al., Science 324, 1421 (2009), A. Gruverman et al., Nano Letters 9, 3539
- [2] A.R. Rocha et al., Physical Review B. 73, 085414 (2006); www.smeagol.tcd.ie.

PS5: Magnetic Properties of Bi_{0.9}La_{0.1}Fe_{0.9}Mn_{0.1}O₃ Films Grown by RF Sputtering

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BiFeO₃ (BFO) is an attractive multiferroic material, which exhibits G-type antiferromagnetic behavior (TN = 380C) and ferroelectric (TC = 810C) properties. Secondary phases, high leakage currents, absence of magnetic hysteresis and unsaturated polarization cycles are among the main problems of BFO thin films. In order to solve these problems, La doping on Bi site and/or Mn doping on Fe site were investigated. Our previous studies on Bi_{0.9}La_{0.1}Fe_{0.9}Mn_{0.1}O₃ bulk ceramics indicated that monophasic samples can be produced showing magnetic hysteresis behaviour. This way we produced a 5 cm ceramic target that was used to grow thin films of Bi_{0.9}La_{0.1}Fe_{0.9}Mn_{0.1}O₃ by RF sputtering

on Pt/Ti/SiO₂/Si substrates. Fixed deposition conditions were RF power (100 W) and pressure (1.2x10⁻² mbar of Argon). Investigation conditions were substrate temperature (400-650C), deposition time (10-60 min) and post-annealing treatments. Single phase thin films were successfully produced, presenting low leakage currents and magnetic hysteresis cycles.

PS6: Antiferromagnetic Ferroelectric State In Half-Doped Manganites: Does It Really Exist?

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We present extensive calculations on magnetic configurations in half-doped (Pr,Ca)MnO₃ (PCMO) within DFT in the GGA+U approximations. The motivation is the prediction by a model [1] that the AF-CE magnetic state, predicted as the most stable for half-doped manganites [2] should exhibit ferroelectricity in the case of almost half doped compounds. The model predicts a sizable charge-ordering on the Mn sites. On the experimental side the P21/m and P21nm lattice structures appear to compete for the ground state at low temperature. An ab initio study of (La,Ca)MnO₃ [3] found that ferroelectric polarization would exist in P21nm due to magnetic symmetry breaking, while in P21/m, being centrosymmetric, it would be present only for specific non-collinear spin arrangements. The ab initio energetics of these structural and magnetic phases compared to others, however, has never been studied. We provide an assessment here for PCMO. We find that in PCMO the AF-CE phase in the low symmetry P21nm structure does indeed show a large electric polarization and an intrinsic Zener-polaron-like ordering of Mn-Mn dimers. However, the low symmetry phase is unstable against relaxation towards the high-symmetry Pbnm: the latter is not polarized and relax to a checkerboard ordering instead. On top of this structural issue, in all cases the AF-CE order turns out to be only metastable, with (at least) AF-A and FM order being lower in energy. The latter magnetic phases are metallic (albeit, in some cases such AF-A, pseudogapped), and cannot support a ferroelectric polarization. We find that charge ordering on Mn sites is almost inexistent, whereas we do observe a pronounced orbital and magnetic-moment ordering involving the eg orbitals of Mn arranged in a zig-zag chain pattern. Interestingly, a similar pattern of magnetization (in modulus) also appears in the others simulated antiferromagnetic structures: AF-A, AF-C and AF-G. In summary, our results rule out the appearance of AF-CE order and its associated ferroelectricity in half-doped PCMO at low temperature. It remains to be verified whether more refined ab initio treatments can change such conclusion. We are currently applying self-interaction-corrected LDA (pSIC) to the same system. Preliminary results so far would seem to confirm the GGA+U results.

[1] D. V. Efremov, J. van der Brink, and D. I. Khomskii, *Nat. Mater.* 3, 853 (2004)

[2] J. B. Goodenough, *Phys. Rev.* 100, 564 (1955)

[3] G. Giovannetti, S. Kumar, J. van den Brink, and S. Picozzi, Phys. Rev. Lett. 103, 037601 (2009). 16

PS7: Structural Effects of Sc Doping on the Multiferroic TbMnO₃

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The new TbMn_{1-x}Sc_xO₃ series has been synthesized and the structural properties have been characterized by x-ray diffraction, neutron diffraction and x-ray absorption spectroscopy. The whole series belongs to the family of ABO₃ perovskites. All samples are isostructural to the parent compound TbMnO₃[1], crystallizing in an orthorhombic cell with space-group Pbnm. The homovalent substitution of Mn³⁺ with the larger Sc³⁺ ion leads to an increase of both the unit cell volume and the BO₆ octahedra tilting. Long range magnetic ordering is not found for x0.3 samples. The analysis of neutron and x-ray diffraction patterns suggest a continuous evolution from a Jahn-Teller distorted BO₆ octahedron in TbMnO₃ into a nearly regular one in TbScO₃. However, x-ray absorption measurements at the Mn K-edge reveal that the local geometry around the Mn³⁺ cation remains distorted in the series even for high values of x. This result is in opposition to previous findings in similar compounds[2] such as LaMn_{1-x}(Ga/Sc)_xO₃ and suggests that the strong orthorhombic distortion of the unit cell due to the small Tb³⁺ cation size favours the stability of the distorted MnO₆ octahedron in diluted systems. This substitution induces a minimum disturbance on the Mn sublattice, the geometrical local structure remains unaltered but magnetic ordering at both Mn and Tb sublattices disappear for small Sc substitution indicating that the magnetic interactions would have a strong directional anisotropy and the Tb ordering is conducted by the Mn ordering.

[1] Kimura T, et al. Nature (London) 2003, 426, 55-58.

[2] Snchez, M. C., et al. Phys Rev. B 2006, 73, 094416.

PS8: Functional Properties of Ba₁₂Fe₂₈Ti₁₅O₈₄ Naturally Self-Assembled Layered System

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A recent study of the BaO-Fe₂O₃-TiO₂ phase diagram found a large number of new phases, with structures featuring moieties from both the polytitanates and hexaferrites, as well as new building blocks showing a mixture of both

phases. One of this mixture phases is the ternary compound with formula $Ba_{12}Fe_{14}Ti_{15}O_{84}$ which was prepared by solid state reaction in the present paper. Phase and crystalline structure analyses carried out by X-ray diffraction indicated a pure monoclinic structure for powders calcined at 12000C/48 h. The HRTEM investigations confirmed the layered nature of the compound and the monoclinic unit cell parameters resulted from XRD analysis. The sintered ceramics show an intrinsic dielectric permittivity of the order of 40-60 at 108-109 Hz and $\tan\delta=0.35$ at 5×10^8 Hz, while at low frequency the apparent permittivity reaches values of 105 due to conduction phenomena. A ferri/ferromagnetic order with coercivity of 40 Oe, remanent magnetisation of 2.5 emu/g and saturation magnetization of 13 emu/g was determined at room temperature, while the thermomagnetic data showed the cancellation of magnetisation at TC 700K.

PS9: Atomic Vapour Deposition (AVD) of Aurivillius Phase Thin Films

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Multiferroic materials possess intriguing properties for novel electronic materials. Layered structures like Aurivillius phase compounds in thin film form provides a promising way to achieve multiferroic properties. In order to achieve high growth rate, excellent control over thickness and Stoichiometry in preparing Aurivillius phase thin films, we are using novel technique called Atomic Vapour Deposition (AVD). The physical and electrical properties of these materials were examined by X-Ray Diffraction (XRD), Scanning electron Microscope (SEM), Atomic Force Microscope (AFM) and Piezoforce Microscope (PFM).

References:

1. Journal of Crystal Growth 272 (2004) 778784
2. Journal of The Electrochemical Society, 152 (2005) 11, F185-F189
3. Chem. Vap. Deposition 14 (2008) 123128

PS10: Thin Film Ferroelectrics By Resonant X-Ray Scattering: Experiment And Simulation

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The characterization of thin film ferroelectric has been done using the resonant x-ray scattering (RXS). This technique combines the spectroscopy and the diffraction techniques and allows us to read the atomic structure of our sample. In this case we have studied thin films of ferroelectric $PbTiO_3$ (PTO), which shows domain ordering. We have also performed reflectivity experiments and

simulations, to study the surface of our samples. Since thin films show new properties compared to bulk materials, Ab-initio calculations of absorption spectra for the PTO ferroelectrics had been done. For the simulations we have used the program FDMNES in order to better understand the electronic structure of the perovskite.

1. Jens Als-Nielsen et Des McMorrow, Elements of Modern X-Ray Physics (Wiley, West Sussex, 2001).
2. Catalan, et al. "Polar Domains in Lead Titanate Films under Tensile Strain", Phys. Rev. Lett. 96 127602 (2006).
3. N. Jaouen, et al. High-pressure dependent ferroelectric phase transition in lead titanate , Phys. Rev. B, 75, 224115 (2007).
4. Fraco Jona et G. Shirane, Ferroelectric crystals(Dover, New York, 1993)
5. N. Spaldin Analogies and Differences between Ferroelectrics and Ferromagnets , and references therein, Physics of Ferroelectrics, Springer, 2007

PS11: Tuning the Atomic and Domain Structure of Epitaxial Films of BiFeO₃

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Thin films of the room-temperature multiferroic BiFeO₃ (BFO) continue revealing interesting properties. Recent works have shown that some domain walls in these films can conduct[1] and it is believed that some of these domain walls can carry net magnetic moment[2]. It is thus important to understand the mechanisms underlying domain formation in the films in order to be able to manipulate the walls. By means of high-resolution x-ray diffraction and piezoforce microscopy we have investigated both the atomic and the domain structure of BFO films grown by pulsed laser deposition under compressive strain on (001)-SrTiO₃, as a function of thickness (d). The films grow forming a coherent interface and sharing the [001] direction with the substrate. The clamping has been observed to exist in two different regimes: ultrathin, d_f 18 nm, and thin, d_f 18 nm. An unusual evolution of the monoclinic lattice parameters with thickness evidences a twinning mechanism that could explain why the 71 degree domain walls are the only ones showing insulating character. We will address several open questions such as the evolution of the electrical polarization with decreasing thickness. The understanding of the exact mechanism for domain formation provides us with a new degree of freedom to control the structure and, thus, the properties of BiFeO₃ thin films[3].

References:

- [1] Seidel et al. NMAT2009
- [2] Martin et al. NANO LET2008
- [3] Daumont et al. PRB2010

PS12: Strain Effects in Spinel Ferrite Thin Films from First Principles Calculations

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We present density functional theory calculations of the structural and magnetic properties of the inverse spinel systems CoFe_2O_4 (CFO) and NiFe_2O_4 (NFO). Both are insulating magnets with high magnetic ordering temperatures and large saturation magnetization, which have been of particular interest over the past few years as building blocks of multiferroic heterostructures [1]. In order to effectively design the magneto-electric response of such multiferroic heterostructures, a clear picture of strain-induced changes in the magnetic properties of CFO and NFO is particularly important. Here we present results for the structural and magnetic properties of both CFO and NFO, with special emphasis on strain-induced changes in the magneto-crystalline anisotropy energy (MAE). Our results are representative for (001)-oriented thin films of CFO and NFO, grown on different lattice-mismatched substrates. We find a large and strongly strain-dependent MAE for CFO, and a significantly smaller but also strongly strain-dependent MAE for NFO. We discuss the influence of cation order within the inverse spinel structure and analyze the effect of different exchange correlation functionals on the structural and magnetic properties. Furthermore, we obtain the magnetoelastic coupling constant B_1 and the magnetostriction coefficient 100 , which are compared to available experimental and other theoretical findings. Our results provide important reference data for analyzing and interpreting experimental results on CFO and NFO thin films.

[1] H. Zheng et al., *Science* 303, 661 (2004).

PS13: Interplay between Magnetic, Structural and Electronic Properties on Ultra-Thin Oxide Films: $\text{FeO}_x/\text{Pt}(111)$

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Ultra-thin oxide films on metals can exhibit unusual properties, which have no counterparts in the corresponding bulk oxide surfaces. The oxide can exist in unusual atomic structures, stabilized by the presence of the substrate underneath. Moreover, upon oxide deposition the work function of the metal substrate may change considerably. We focus in particular on the properties of iron oxides ultra-thin films deposited on $\text{Pt}(111)$, which have been extensively characterized experimentally in the past. By means of first principle DFT+U calculations, we highlight the coupling between structural, magnetic and electronic properties in a $\text{FeO}_x/\text{Pt}(111)$ film as a function of the oxygen chemical potential.[1] We have identified the principal mechanisms for the structural and electronic non-homogeneous characteristics observed in the Moir unit cell formed between oxide film and metal support, due to the lattice mismatch between $\text{Pt}(111)$ and the FeO film, coherent with the most recent experimental findings.[2,3,4]

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PS14: Calculations and Experimental Values of Hyperfine Parameters in Multiferroic Manganites: Electric Field Gradient and Hyperfine Magnetic Field

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The manganites RMnO₃ are a current topic of research due to the interesting interplay of orders (lattice, spin, orbital, charge) resulting in effects such as colossal magnetoresistance and multiferroism. The hyperfine parameters, electric field gradient (EFG) and magnetic hyperfine field, highly sensitive to the neighbouring charge density, can be used in the experiments to probe local atomic environments. The EFG has been previously related experimentally to the electric polarization, so that its accurate measurement, or calculation, is relevant to the study of multiferroic manganites. Density functional theory (DFT) calculation can be compared with experiments to help in its interpretation. We report DFT calculations with the full potential linear augmented plane wave method implementation. The hyperfine parameters are studied in a series of rare-earth (La, Pr, Y, Eu, Gd, Ho, Er, Yb) and alkaline-earth (Ca, Sr, Ba) compounds with respect to the structure, magnetism and electronic band-structure. A comparison with experimental results obtained by the Perturbed Angular Correlation hyperfine technique is presented.

PS15: Magnetic and Structural Properties of Multiferroic Systems AlFeO₃ ; GaFeO₃

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Materials where spontaneous magnetic and electric polarization coexist are of great interest for both new electronic devices conception as for fundamental viewpoint. One interesting path is to analyse the origin of coupling between charge, spin and orbital degrees of freedom. In this work, we investigate multiferroic magnetoelectric systems AlFeO₃, GaFeO₃. Ferroelectricity is caused

by non centro-symmetric structure but the nature of the magnetism has not been successfully understand. We also present an extended study of parent compounds $\text{Al}_{2-x}\text{Fe}_x\text{O}_3$ and $\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$ ($0 < x < 0.2$). With doping, the interactions between iron spins increase, leading to ferromagnetic, ferrimagnetic or antiferromagnetic order. This magnetic study is made by local EPR measurements coupled with magnetization data on polycrystalline samples. Disorder in the distribution of the iron sites seems to have impact on the magnetic properties and for this reason we also focus our study on crystal structure by means of ^{27}Al and ^{71}Ga NMR compared to DRX measurements.

PS16: Spin Dynamics of the Frustrated Diluted Magnetic Semiconductors ZnMnSe and CdMnTe

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The magnetic properties of the diluted magnetic semiconductors ZnMnSe and CdMnTe have been investigated by means of density functional theory calculations and spin dynamics simulations. The concentration range of Mn-doping was 25-50%. The electronic structure calculations are performed with the TB-LMTO scheme and the coherent potential approximation. A LDA+U exchange-correlation functional was used with a Hubbard U on the Mn 3d-states. It is found that for a given magnetic reference state, ferromagnetic or disordered local moments, the exchange interactions depend only weakly on the gap of the electronic states. We argue that for a larger gap the influence of gap-size is small and the most important is p-d coupling of Mn-t₂ and Te-p states for occupied states. Superexchange is suppressed by the size of the gap. Spin dynamics simulations [1] were performed at temperatures above and below the magnetic ordering temperature. As been established in experiments, CdMnTe and ZnMnSe -alloys show spin glass behavior for concentrations below the nearest-neighbour percolation limit [2,3]. The effect of frustrations has been investigated by sampling of correlation functions in real and reciprocal space. Simulations were made following a quenching protocol, starting with the magnetization in a high temperature state and setting the temperature to a lower temperature at the start of the simulation. We investigate the trends for how the correlations evolve in time for a range of different chemical compositions of the sample. It is established that short range correlations are present also above the spin glass temperature.

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PS17: Composition Dependence of Magnetoelectric Coupling in Y type Hexagonal Ferrite $\text{Ba}_{2-x}\text{Sr}_x\text{Ni}_2\text{Fe}_{12}\text{O}_{22}$

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Study of magneto-electric multiferroics has become a hot topic in physics and technology. These materials have attracted interest as next generation devices. However, there are some problems for actual applications, e.g., too low working temperatures, leaky behaviors at high temperature, and weak coupling between magnetism and ferroelectricity. Recently, it was discovered that some manner of spiral magnetic structures induce ferroelectricity [1]. In such ferroelectrics, strong couplings between magnetism and ferroelectricity can be expected. Hexagonal ferrite system, which has various magnetic ordered states above room temperature, is one of promising candidates to solve these problems. We have grown single crystal of Y type hexagonal ferrite $\text{Ba}_{2-x}\text{Sr}_x\text{Ni}_2\text{Fe}_{12}\text{O}_{22}$ and measured their magnetic and electric properties. The $x=0$ sample show just a simple ferrimagnetic behavior and don't show ferroelectricity. However, it was observed that introducing Sr into Ba site makes the interaction between stacked layers antiferromagnetic. Therefore, with increasing x , the ground state changes from ferrimagnetism to antiferromagnetism, and then magnetically-induced ferroelectricity appears by applying magnetic fields to perpendicular to the hexagonal c axis for $x \neq 0$ samples. In this presentation, we will discuss the x dependence of magnetoelectric coupling in the hexagonal ferrite system.

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PS18: Switching Dynamics of The Magnetically Induced Ferroelectric Polarization in MnWO_4

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Coexisting ferroic orders become interesting when there is a pronounced interaction between them. Especially an interaction between electric and magnetic order is highly desirable for device applications. However, in split-order parameter multiferroics where magnetic and ferroelectric order emerge independently, their coupling is in general weak. Contrary, in joint-order parameter multiferroics one order is induced by the other and therefore the coupling is intrinsically strong. An example is MnWO_4 where the ferroelectric polarization is induced by a spin spiral. By applying an electric field we can transform the sample to an electric as well as magnetic single-domain state. Here we performed time-resolved optical second harmonic generation (SHG) measurements of this switching process. Despite the great interest in switching a magnetization by an electric field nothing is known about the progression of the switching process. We present the dependence of the switching process on the amplitude and pulse length of the applied electric field. Furthermore, it is still unclear if the origin of the polarization is electronic or ionic. Since the displacements of the

charges are small, structural analysis techniques cannot resolve them and thus cannot uniquely distinguish between electronic and ionic displacements. The large SHG efficiency in spin-spiral induced ferroelectrics points to an electronic contribution. Future investigation of the dynamics of the switching process can contribute to further clarify this open question.

PS20: Design of Magnetic Ferroelectrics: La₂(Ti,Mn)₂O₇.

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We propose the magnetic doping of structural ferroelectrics as an alternate route towards materials with coexisting magnetism and ferroelectricity. Our initial case study is La₂Ti₂O₇, a monoclinic structure produced by oxygen layer intercalation in a periodic stacking of four perovskite blocks [1]. La₂Ti₂O₇ is a robust ferroelectric with a unique polarization axis, high critical temperature (1800 K) [2], saturation polarization (5 $\mu\text{C}/\text{cm}^2$) and coercive field (45 kV/cm). We verified that that La₂Ti₂O₇ is a band insulator with DFT-GGA calculated gap of 2.8 eV. Berry-phase polarization calculations reproduce well the experimental polarization (calculated value 6.6 C/cm²). We then substitute Mn for Ti realizing La₂(Ti_{1-x}Mn_x)₂O₇ at various x. Mn adopts the same valency +4 as Ti, but in a t₃ magnetic configuration. The material thus remains a band insulator while becoming magnetic. Exploring a number of magnetic configurations for x=1 (i.e. for La₂Mn₂O₇), x=0.25 and x=0.125, we indeed find stable antiferromagnetic phases of various degrees of complexity. In all these magnetic states, ferroelectricity survives largely unscathed (P 6 C/cm²). The antiferromagnetic order is (from total energy differences) rather weak; this is to some extent expected from the dominant superexchange interaction between t₃ orbitals. We are now further pursuing this idea with other transition-metal substitutions of potentially mixed-valent behavior.

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PS21: A Comparison between Ferromagnetic and Multiferroic Nanoparticles-Based-System for Drug Delivery

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The aims of this work is to study multiferroics nanoparticles (MNPs) based-systems for drug delivery. Nowadays, drug delivery system are based on ferromagnetic nanoparticles (FNPs) (i.e. $\gamma\text{-Fe}_2\text{O}_3$) in the range of 50-300 nm, driven by external magnetic field gradients. The goal is to find out whether MNPs can be used instead of FNPs in a system driven by magnetic and electric fields. We

review the application and the physical principles underlying FNP, and discuss the capabilities of MNP for drug delivery.

PS22 Ferroelectricity Enhancement Induced by Magnetic Ordering in Multiferroic BiMn7O12

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The family of manganites displaying quadruple perovskite structure (general formula AMn_7O_{12}) is extremely interesting due to its structural complexity allowing the direct observation of charge, orbital and spin orders. The synthesis takes place in high pressure / high temperature conditions, making of these compounds metastable systems at room conditions. In $BiMn_7O_{12}$, the presence of the bismuth 6s2 lone pair causes a symmetry breaking, never observed in the other known quadruple perovskites, at the origin of room temperature ferroelectricity. Two different magnetic transitions are observed at lower temperatures, corresponding to the ordering of two independent manganese sublattices. Below 55 K the setting of nonzero magnetization is detected, ascribed to the presence of Dzyaloshinskii-Moriya (DM) interaction, yielding a slight deviation from the purely AFM order determined by powder neutron diffraction. Two peaks observed in the dielectric permittivity matching the magnetic ordering transitions suggest the presence of ferroic coupling, confirmed by the detection of a structural anomaly taking place at 55 K, involving an increase of the cell volume, and consequently the enhancement of the dipole moment.

PS23: Effects of Substitutions in the Delafossite CuCrO2

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The delafossite systems ABO_2 have been recently extensively studied because of the discovery of spin driven ferroelectricity in $CuFeO_2$ [1]. Numerous studies were also devoted to the chromium compound $CuCrO_2$ which presents likewise multiferroic properties [2]. It crystallizes in the delafossite structure ($R\bar{3}m$), which consists of an alternative stacking along the c axis of edge-shared $Cr^{3+}O_6$ octahedra separated by layers of Cu^+ . This anisotropic structure and the frustrated triangular lattice of chromium lead to a complex magnetic ordering. Below $T_N = 24$ K, the magnetic structure is an incommensurate helicoidal spiral $(q \ q \ 0)$ $q=0.329$ and induces a ferroelectric polarization at T_N

[2]; moreover this 3D magnetic order exhibits a short coherence length along c [3]. Substitution effects on the different sites is worth to be studied as B site substitution by a non magnetic cation (Al, Ga, Rh) in CuFeO₂ is known to induce a change in the magnetic behavior, responsible for the appearance of polarization. In contrast, for CuCrO₂ the magnetic dilution by 2%– Mg does not change the magnetic structure [3], and the measured polarization in Al-substituted ceramic samples decreases from 19 to 8.5 C/m² for $x_{Al} = 0$ and $x_{Al} = 0.10$, respectively. Moreover, A site substitution could affect the 3D magnetic ordering via the O-A-O linkages. Ag⁺ is a good element for that as AgCrO₂ is isostructural to CuCrO₂, with the same delafossite R-3m structure and electric polarization concurrent with a helicoidal magnetic order ($q \parallel c$), $q = 0.327$ at $T_N = 21\text{K}$ [2]. Complete substitution at the oxygen site has been also made with sulphur. AgCrS₂ has a different structure (R3m), the polyhedra around A and B are different, compared to CuCrO₂, leading thus to different ligand-metal orbital hybridisation, although polarization has been measured on AgCrS₂ (20 C/m² below $T_N=40\text{K}$) [4].

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PS24: Electric-Field Effects on Spin Modes in BiFeO₃ Crystal

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We have detected by Raman scattering two species of spin propagation modes (magnon) in BiFeO₃ single crystal: in-plane (ϕ mode) and out of cycloidal plane (ψ mode) modes. The frequencies of these modes have been successfully compared to the results of a Ginzburg-Landau mode. This result shows that the magnon modes might be interpreted as electromagnon. Low temperature measurements reveal simultaneous anomalies associated with the spin re-orientation in the frequencies and intensities of the magnon and the E1 polar phonon modes. In order to characterize the magnetoelectric coupling, an external electric field has been applied. The frequencies of the ϕ modes strongly increase with the voltage in an opposite way of the ψ modes. The shifts have been correlated with the polarization cycle. We show a linear relation between the frequency shift of magnons and of the E1 phonon.

PS25: Observation of Magnon in TbMnO₃ by Raman Scattering

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Magnetic excitations in the multiferroic TbMnO₃ have been investigated by Raman spectroscopy. Our observations reveal spin excitations at 30 cm⁻¹ and at 60 cm⁻¹. The energies of these magnon modes correspond to the ones of the electromagnons observed by IR transmission spectroscopy. The magnon modes measured by Raman scattering are only observed in the cycloidal phase below the Curie temperature. Our data show that both excitations have not a pure magnetic activity. The mode at 60 cm⁻¹ is interpreted as the zone-edge magnon. Moreover, the 30 cm⁻¹ magnon mode is enhanced when the electric field of light E is along the spontaneous polarization (c axis). The Raman selection rules for this mode show its complex origin. To explain this mode the Dzyaloshinskii-Moriya interaction and a model based on cross-coupling between magnetostriction and spin-orbit interaction have been proposed.

PS26: Study of Multiferroic Properties of Ga_{2-x}Fe_xO₃ (0.8 ≤ x ≤ 1.2)

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Materials that simultaneously show electric and magnetic ordering are gaining much attention due to the promising multifunctional device applications and because of interesting physics as well. GaFeO₃ (GFO) that exhibits piezoelectricity and ferrimagnetism is considered to be a very promising multiferroic material for the following reasons: (i) its TC is of about 200 K and may be increased to values close to the room temperature by increasing the Fe content (x) of Ga_{2-x}Fe_xO₃ (TC = 350 K for x=1.4), controlling the site disorder between Ga and Fe with different preparation methods etc., (ii) it is relatively easy to prepare single phase GFO samples with the conventional solid state route and (iii) is considered to be environmental and social friendly when compared to most of the other lead and bismuth based magnetoelectric materials. Excess Fe atoms occupying the octahedral Ga sites are ferromagnetically coupled with the Fe atom at one of the two Fe sites, which results in the net magnetic moments observed in the experiments. In the present work, we have prepared polycrystalline Ga_{2-x}Fe_xO₃ samples. Structural studies are done using X-Ray Diffraction and Rietveld refinement. Magnetic properties are studied using low temperature high magnetic field Mossbauer spectroscopy, Neutron Diffraction and VSM. Dielectric, P-E and resistivity measurements have been done to reveal the electric properties. It is observed that change in cation distribution with the off stoichiometry of Gallium and Iron drastically alter the magnetic and electric properties of the compound. Raman Spectroscopy is used to throw light on the issue of spin-phonon coupling which has not yet been explored for this sample.

PS27: Cation site-disorder, magnetic ordering and phonons in FeAlO₃: A first-principles Study

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FeAlO₃, reported to have ferrimagnetic and piezoelectric properties, has cation sites with both tetrahedral and octahedral coordination. Motivated by the rich set of its observed properties, we use first-principles density functional theory based calculations to determine the coupling between cation (Fe-Al) site-disorder and its magnetic ordering and vibrational properties. Using microscopic information available from our calculations, we attempt to investigate the possibility of magneto-relaxor behavior with Ga substitution at Al site.

PS28: Magnetodielectric Studies of Different Delafossite Multiferroics

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Oxide materials are the most fascinating and exciting class of materials with a variety of interesting phenomena such as ferroelectricity, superconductivity, colossal magnetoresistance (CMR) and multiferroicity. The ternary triangular-lattice antiferromagnet (TLA) ABO₂ system is the most obvious example of geometrically frustrated magnetic system. A large number of ternary noble metal oxides crystallize as ABO₂ type delafossite structure [1,2]. The CuFeO₂, CuCrO₂, and AgCrO₂ order antiferromagnetically and insulators and multiferroics at low temperature [3,4]. CuFeO₂ shows ferroelectricity only in the presence of magnetic field between 7 to 12T and only in the noncollinear incommensurate phase. However, the different nonmagnetic substitution (Al, Ga and Rh) at Fe site leads to modify the magnetic structure and hence, responsible for ferroelectricity even in the absence of magnetic field. ACrO₂ (A=Cu and Ag) are isospin and isostructural and showing the spin driven ferroelectricity upto TN, 24K and 21K, respectively, for Cu and Ag [4]. The magnetodielectric studies of above mention polycrystalline delafossites has been investigated. In polycrystalline, the contribution in magnetodielectric comes from the sum of all orientations. All these delafossites show symmetric and butterfly wing like behaviour with increasing and decreasing magnetic field. The maximum effect can be observed near TN. After analysing these data one can obtain a clear peak at TN, irrespective of the different origin of polarization in CuFeO₂ and ACrO₂.

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PS29: Enhanced Multiferroic Properties of BiFeO₃ Ceramics on La and Pr Substitution at A Site.

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Here, we report the enhancement in multiferroic properties of Perovskite Bi_{1-x}La_xFeO₃ (0.0 < x < 0.3) oxides on the substitution of high valence Pr at A site. The bulk samples were prepared by a sol-gel method. The crystal structure examined by X-ray powder diffraction indicates that the samples were single-phase and crystallize in a rhombohedral (space group, R-3c) structure. The structural phase transition from rhombohedral to orthorhombic phase was observed at x = 0.20. The multiferroic properties of La doped BiFeO₃ were studied and further remarkable increase in multiferroic properties has been observed as a result of Pr doping (in Bi_{1-x}La_xFeO₃, x=0.2). Pr doping significantly increases the resistivity and leads to a successful observation of electrical polarization hysteresis loops. All the samples have been found to possess a spontaneous magnetic moment at room temperature which increases further at low temperatures. The strong dependence of remnant polarization and dielectric constant on the strength of magnetic field is a direct evidence of magnetoelectric coupling in Bi_{1-x}La_xFeO₃, x=0.2 ceramics.

PS30: Hybrid Functional Studies of Multiferroics

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Recently, hybrid Fock exchange/density functional theory functionals have received great attention in the solid state community. In particular, the HSE (Heyd-Scuseria-Ernzerhof) screened hybrid functional, widely applied in solid state calculations[1], becoming a new computational paradigm for accurate electronic structure calculations of complex materials. In fact, HSE has been recently applied to solid states systems and has shown very good performance with respect to standard local DFT approaches, especially for insulating and correlated systems. Despite this, very few studies exist in the multiferroic field, and clearly much work is needed in order to assess the performance of HSE in this recent field of material research. In this framework, we focus on two prototypical systems such as BiFeO₃ (BFO) and HoMnO₃ (HMO). We perform an accurate study of the structural, electronic, magnetic and ferroelectric properties based on the comparison of the performance of standard DFT approaches, and more advanced and recent hybrid-DFT, such HSE. Furthermore, we have focussed

on Dysprosium-Orthoferrite, DyFeO₃, which was recently suggested from experiments to show an induced multiferroic phase.[2] By performing accurate ab-initio density functional calculations, we focused on the mechanism at the basis of the polar behavior. For BFO and HMO, by comparing our calculations with available experimental data, our study points towards a truly realistic description of multifunctional materials, such as multiferroics. For BFO, we also included state-of-the-art GW calculations, which, to the best of our knowledge, have not yet been done. They show that HSE approach already account well for the electronic structure of these materials. For DFO, we confirm in particular that Dy-4f electrons, more-often-than-not neglected in modelling studies, play an important role in stabilizing the magnetic-field-induced ferroelectric state of DyFeO₃, as recently suggested by experimental work[2]. The estimated electric polarization, in good agreement with experiments, shows an unexpectedly large magnitude (0.1-0.2 $\mu\text{C}/\text{cm}^2$). A careful electronic structure analysis suggests that coupling between Dy and Fe spin sublattices is mediated by Dy-d and O-2p hybridization. Our findings indicate that the interaction between the f and d sublattice might be used to tailor ferroelectric and magnetic properties of multiferroic compounds. From the methodological point of view, Dy-ferrite represent a nice benchmark for the theoretical treatment of 4f electrons. Our results are shown to be robust with respect to the different state-of-the-art computational schemes used for d and f localized states, such as the DFT+U method, the HSE hybrid functional, and the GW approach.

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PS31: Ferroelectricity in Sb₂S₃ Nanowire Arrays

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Sb₂S₃ is semiconducting as well as a weak ferroelectric material, which exhibits phase transitions at 310 K and 420 K, associated with small structural changes in the coordination sphere of antimony atoms.¹ Although the synthesis of various types of Sb₂S₃ nanostructures have been the basis of numerous studies, no work has been reported so far on the preparation of arrays of Sb₂S₃ nanowires and their ferroelectric characteristics. Here we employed an anodic aluminium oxide (AAO) template² to prepare arrays of Sb₂S₃ nanowires and

study their ferroelectric and piezoelectric properties using a switching spectroscopy piezoresponse force microscopy (SS-PFM). SS-PFM results indicate individual Sb₂S₃ nanowire exhibit piezo and ferroelectric response.

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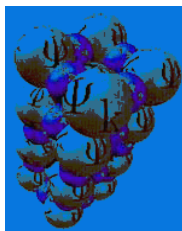
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21. Gabriella Maria De Luca, CNR-SPIN, Italy
22. Nitin Deepak, Tyndall National Institute, India
23. Kris Delaney, Univ. California Santa Barbara, USA
24. Flavia Viola Di Girolamo, Federico II University, Naples, Italy
25. Domenico Di Sante, Univ. L'Aquila, Italy

26. Kathrin Dörr, IFW-Leibniz Institut Dresden, Germany
27. Luca DOrtenzi, University of LAquila, Italy
28. Claude Ederer, Trinity College Dublin, Ireland
29. Marta Elzo Aizarna, Institut Nel CNRS (Grenoble), France
30. Saeedeh Farokhipoor, Zernike Institute (Rug university), Netherland
31. Josep Fontcuberta, Institut de ciencia de Materials, (ICMAB)-CSIC Spain
32. Daniel Fritsch, Trinity College Dublin, Ireland
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34. Stéphane Fusil, Unit Mixte de Physique, CNRS/Thales, France
35. Livia Giordano, Univerista Di Milano-Bicocca, Italy
36. Joo (Nuno Santos) Goncalves, Universidade de Aveiro, Portugal
37. Christoph Gruber, TU Vienna, Austria
38. Gisele Gruener, LEMA / Facult des Sciences, France
39. Alexander Hearmon, University of Oxford, United Kingdom
40. Johan Hellsvik, Uppsala University, Sweden
41. Jeroen Heuver, Zernike institute for advanced materials, Netherland
42. Yuji Hiraoka, Osaka University, Japan
43. Tim Hoffmann, University of Bonn, Germany
44. Jiawang Hong, Rutgers Univ., USA
45. Tanveer Hussain, Univ. Uppsala, Sweden
46. Diana Iusan, Univ. Uppsala, Sweden
47. Adam Jacobsson, Forschungszentrum Juelich, Germany
48. Daniel Khomskii, Universitaet zu Koeln, Germany
49. Marjana Lezaic, Forschungszentrum Juelich, Germany
50. Jia Liu, North Carolina State Univ., USA
51. Giorgia Maria Lopez, Univ. of Cagliari and Cnr-Iom, Cagliari, Italy
52. Luca Matteo Martini, Universit degli Studi di Trento, Italy
53. Shlomi Matityahu, University of the Negev, Israel

54. Ingrid Mertig, MPI für Mikrostrukturphysik Halle and M. Luther Universität Halle- Wittenberg, Germany
55. Francesco Mezzadri, Università degli Studi di Parma, Italy
56. Joel Moore, University of California Berkeley, United States
57. Elise Pachoud, Laboratoire CRISMAT, France
58. Krisztian Palotas, Univ. Budapest, Hungary
59. Jonathan Peace, University of Warwick, United Kingdom
60. Silvia Picozzi, CNR-SPIN L'Aquila, Italy
61. Daniele Preziosi, CNR-SPIN, Italy
62. Danilo Puggioni, UNiv. Cagliari, Italy
63. Carmen Quiroga Rodriguez, LMU Munich, Germany
64. Kouros Rahmizadeh, Forschungszentrum Juelich, Germany
65. Abdulrafu Raji, Univ. Cape Town, South Africa
66. Muhammad Riaz, CNR-SPIN, Italy
67. Mirko Rocci, Universidad Complutense de Madrid, Spain
68. James Rondinelli, Argonne Natl.Lab, USA
69. Pauline Rovillain, Université Paris 7, France
70. Konstantin Rushchanskii, Forschungszentrum Juelich, Germany
71. Tanusri Saha-Dasgupta, Bose Natl. Center, India
72. Andrea Scaramucci, Univ Groningen, The Netherlands
73. Martin Schlipf, Forschungszentrum Juelich, Germany
74. Sharmila Shirodkar, Jawaharlal Nehru Centre for Advanced Scientific Res, India
75. Oleksandr Shvets, University of Groningen, Netherlands
76. Virginie Simonet, Institut Néel CNRS Grenoble, France
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78. Ivetta Slipukhina, Forschungszentrum Juelich, Germany
79. Alessandro Stroppa, CNR-SPIN L'Aquila, Italy
80. Jean-Marc Triscone, Université de Genève, Switzerland

81. Alexey Ushakov, University of Cologne, Germany
82. Ruggero Vaglio, -SPIN Genova, Italy
83. Jeroen van den Brink, IFW-Leibniz Institut Dresden, Germany
84. Maria Varela, Oak Ridge National Lab, United States
85. Justin Varghese, Tyndall National Institute, Ireland
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Psi-k Network : Towards Atomistic Materials Design



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PSI-K WORKSHOP FINANCE REPORT

Title of the Workshop	European School on Multiferroics 2010 (ESMF 2010)
Workshop Organisers	Silvia PICOZZI (CNR-SPIN, L'Aquila IT), Jeroen VAN DEN BRINK (IFW Dresden DE), Laurent CHAPON (ISIS Rutherford Lab UK), Manuel BIBES (CNRS FR)
Location of the Workshop	Faculty of Science, University of L'Aquila – COPPITO L'AQUILA (ITALY)
Dates of the Workshop	Sept. 26 th – Oct. 1 st 2010
Total Grant from Psi-k	€ 6.200,00

EXPENDITURE

WORKSHOP DELEGATES / SPEAKERS			
Name and Country of Claimant	Travel	Accommodation	Total (€'s)
TRISCONE Jean Marc (Geneva CH)	€	€ 140,00	€ 140,00
COEY John (Dublin IE)		€ 140,00	€ 140,00
MOORE Joel (Berkeley USA)		€ 140,00	€ 140,00
SIMONET Virginie (Grenoble FR)		€ 210,00	€ 210,00
VARELA Maria (Oak Ridge USA)		€ 280,00	€ 280,00
DÖRR Katrin (Dresden DE)		€ 350,00	€ 350,00
CHAPON Laurent (Didcot, UK)		€ 350,00	€ 350,00
VAN DEN BRINK Jeroen (Dresden, DE)		€ 350,00	€ 350,00
BIBES Manuel (Palaiseaux, FR)		€ 225,00	€ 225,00
FUSIL Stéphane (Palaiseaux, FR)		€ 225,00	€ 225,00
KHOMSKII Daniel (Koeln, DE)		€ 420,00	€ 420,00
BOMBARDI Alessandro (Didcot, UK)		€ 350,00	€ 350,00
CHEONG Sang-Wook (New York, USA)		€ 280,00	€ 280,00
MERTING Ingrid (Wittemberg, DE)		€ 140,00	€ 140,00
Fontcuberta Josep (Barcelona ES)		€ 70,00	€ 70,00
Total Travel & Accommodation			€ 3.670,00

WORKSHOP REFRESHMENTS / CONFERENCE DINNERS			
Date	Tea / Coffee	Lunch / Dinner	Total (€'s)
September 27 th – October 1 st , 2010		€ 1.867,75	€ 1.867,75
September 29 th , 2010		€ 462,25	€ 462,25
Total Refreshments			€ 2.330,00

MISCELLANEOUS EXPENDITURE	
Details	Total (€'s)
Welcome meeting + hotel conference room (including soft drink for participants - Sept 26 th , 2010)	€ 200,00
Total Miscellaneous	€ 200,00
Total Travel & Accommodation	€ 3.670,00
Total Refreshments	€ 2.330,00
Total Miscellaneous	€ 200,00
TOTAL EXPENDITURE	€ 6.200,00