Multifunctional Oxides: Synergy between fundamental science and novel technologies

December 13th-15th 2017, Argentina

GENERAL PROGRAM

PROGRAM

	Wed 13/12	**Thu 14/12**	**Fri 15/12**
9:00	Inscription - Opening	**Plenary 3: A. Barthelemy**	**Plenary 6: M. Aguirre**
9:50	**Plenary 1: S. Menzel**	**Plenary 4: G. Herranz**	**Plenary 7: J. Briático**
10:40	N. Ghenzi	M. Stachiotti	J. Sacanell
11:10	BREAK	BREAK	BREAK
11:30	D. Rubi	R. Carbonio	R. Fuentes
12:00	M. Linares	V. Vildosola	G. Leyva
12:30	LUNCH	LUNCH	LUNCH
14:30	**Plenary 2: M. Rozenberg**	**Plenary 5: M. Mostovoy**	**Round tables**
15:20	D. Comedi	S. Carreira	
15:50	M. Quintero	N. Massa	
16:20	BREAK	BREAK	
17:00	DISCUSSION-POSTERS	DISCUSSION-POSTERS	CLOSING

PLENARY TALK ABSTRACTS

Dr. Stephan Menzel - Forschungszentrum Jülich - Germany
"Switching Dynamics, Limiting Processes and Parasitic Effects in Resistive Switching Devices based on the Valence Change Mechanism"

Dr. Marcelo Rozenberg - Univ. Paris Sud - France
"Neuromorphic electronic behavior in transition metal oxides systems"

Dr. Agnes Barthelemy - CNRS/Thales - France
"Potential of the LaAlO3/SrTiO3 interface for spintronics"

Dr. Gervasi Herranz - ICMAB - Spain
"Opportunities of multifunctional materials in energy efficient oxide electronics"

Dr. Maxim Mostovoy - University of Groningen - Netherlands
"Electric control of topological defects in magnets"

Dr. Myriam Aguirre - Univ. Zaragoza - Spain
"Material development and nanostructure optimization for devices based on thermoelectric and thermomagnetic phenomena"

Dr. Javier Briático - CNRS/Thales - France
"HTc superconductor-based devices: low consumption-high performance applications"

Switching Dynamics, Limiting Processes and Parasitic Effects in Resistive Switching Devices based on the Valence Change Mechanism

S. Menzel[1], A. Marchewka[2], C. Funck[2], C. La Torre[2], K. Fleck[2], B. Rösgen[1], V. Havel[1], C. Bäumer[1], W. Kim[1], A. Schönhals[2], M. von Witzleben[2], S. Hoffmann-Eifert[1], V. Rana[1], R. Waser[1,2], R. Dittmann[1], D. J. Wouters[2], U. Böttger[1]

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Resistive switching devices based on the valence change mechanism (VCM) are a possible candidate for future use in non-volatile memory and neuromorphic applications. VCM cells can be switched between a low resistive state (LRS) and a high resistive state (HRS) by applying voltage pulses with opposite polarities. The transition from the HRS to the LRS is called SET process and the reverse transition is called RESET process. The VCM switching mechanism in n-type transition metal oxides is based on the motion of ionic defects (typically oxygen vacancies) that act as donors. The oxygen vacancies increase the local electron density and modulate the electrostatic barrier at the metal/oxide interfaces in the metal/oxide/metal device stack.

In this talk, experimental studies combined with device modeling will be presented aiming at the understanding of the dynamic VCM switching process. The current transport mechanism of $Pt/SrTiO_3/Nb:SrTiO_3$ devices will be discussed. Current transport measurements of this device show different temperature dependence in the high and low voltage regime. To explain this feature, electronic transport calculations using density functional theory (DFT) combined with the non-equilibrium Green's function formalism and drift-diffusion continuum methods were employed. The analysis of the simulation results confirm the importance of the electrostatic barrier for explaining the current transport and allow for an explanation of the observed experimental behavior. The dynamics of the SET and RESET transition were investigated using pulse measurements with varying pulse amplitudes over many orders of magnitude in time and ambient temperature. The experimental results show that a gradual switching precedes the typical abrupt SET event. Comparison with dynamic compact modeling results reveals that both gradual and abrupt switching originate from the thermally accelerated drift of oxygen vacancies, which leads to a thermal runaway. Using dedicated coplanar wave guide devices switching in the sub-ns regime is feasible. In this regime, the switching time is still limited by the measurement setup and not by an intrinsic speed limit. The measured gradual RESET transition, in contrast, can be explained in terms of a drift-diffusion balance by means of simulation. Due to this balance a unique equilibrium state can be reached, which is independent of the initial state. Moreover, it will be discussed how oxygen exchange reactions at the two interfaces influence the switching dynamics. Depending on the

interface, the oxygen exchange reactions could lead to an enhanced RESET or to the occurrence of parasitic switching loops.

Neuromorphic electronic behavior in transition metal oxides systems

Marcelo Rozenberg

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CNRS - Universite Paris-Sud

The information age we live in is supported on a physical under-layer of electronic hardware, which originates in condensed matter physics research. The mighty progress made in silicon based technology seemed endless. However, with the smallest feature size of transistors reaching down to mere 5 nm, this technology is reaching an unavoidable physical limit. This calls for exploration of new alternatives. Neuromorphic inspired systems are making fast progress. But this is based either on dedicated hardware made with conventional electronics, or in software, such Deep Neural Networks, running in conventional computers. Resistive switching phenomena opens the way to explore a technological disruptive solution, namely, implement simple devices with the required functionalities to directly build neuromorphic systems. In this talk we shall describe recent efforts towards making artificial neuron and synapses using transition metal oxides, including Mott strongly correlated systems.

Potential of the $LaAlO_3/SrTiO_3$ interface for spintronics

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The interface formed by an $LaAlO_3$ thin film grown on top of a TiO_2-terminated $SrTiO_3$ substrate hosts a two-dimensional electronic system [1]. Although controversy exists regarding some of its physical properties and their precise origin, it is universally found that conductivity only appears beyond an $LaAlO_3$ thickness threshold of 4 unit cells [2] which is a stringent limitation for efficient tunneling application [3]. Through magnetotransport and X-ray absorption spectroscopy experiments, we will show that this critical thickness can be reduced to just one unit cell when a metallic film of cobalt is deposited on top of $LaAlO_3$ [4]. We will demonstrate the generality of the observed onset of conductivity below the critical thickness of $LaAlO_3$ in on Metal/$LaAlO_3$/$SrTiO_3$ heterostructures, as recently predicted by first-principles calculations [5] and in link with the work function of the metal and enthalpy of formation of the oxide [6].

The large Rashba spin-orbit coupling present at the interface could be exploit for spin to charge interconversion, which present advantages for future spintronics. We will show spin pumping experiments that evidence a very large spin to charge conversion efficiency of the 2DEG through the inverse Edelstein effect. This effect can be modulated by a gate voltage and its variation is interpreted in terms of a crossover between the occupancy of one to several bands with different orbital characters and different spin-orbit textures [7]. This suggest that oxide interfaces have a strong potential for spintronics, both for the generation or detection of spin currents.

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[3] N. Reyren *et al*., Phys. Rev. Lett. 108, 186802 (2012).
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[5] R. Arras *et al.*; Phys. Rev. B 85, 125404 (2012).
[6] D. Vaz et al.; Adv. mat.. 29, 1700486 (2017).
[7] E. Lesne et al.; Nat. Mat. 4726 (2016).

Opportunities of multifunctional materials in energy-efficient oxide electronics

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Multifunctional materials and, in particular, ferroelectric and magnetic metal oxides, offer opportunities to develop novel device concepts for energy-efficient data storage and advanced computing. Bearing in mind these prospects, we are focusing our research on different solutions to the demands for energy-saving technologies, targeting at integrating functional oxides on technological platforms, particularly silicon and flexible substrates. Our activities embrace several topics: (i) Spintronic devices exploiting spin currents for efficient magnetization switching and electric control of spin waves to develop dissipationless spintronic logic circuits. (ii) Ferroelectric junction devices towards neuromorphic-like computing and pattern recognition. (iii) New materials and concepts for photovoltaics, implying both the use of ferroelectric materials as well as innovative plasmonic concepts to enhance the photovoltaic responses.

Electric control of topological defects in magnets

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Complex interplay between charge, spin, orbital and lattice degrees of freedom in transition metal oxides gives rise to new functionalities and fascinating physical phenomena, such as high-temperature superconductivity and colossal magnetoresistance. In my talk I will focus on multiferroic materials with coexisting orders of electric and magnetic dipoles allowing for the electric-field control of magnetization and electric excitation of spin waves, which may find many technological applications. Magnetoelectric switching crucially depends on the dual nature of topological defects in multiferroics, such as the domain walls in rare earth orthoferrites that are both ferroelectric and ferromagnetic or the discrete vortices in hexagonal manganites with coupled structural, ferroelectric and magnetic order parameters.

More complex topological defects, skyrmions, have been recently discovered in chiral itinerant magnets and multiferroic Mott insulators. The non-coplanar skyrmion spins induce effective electromagnetic fields acting on electrons and magnons, and resulting in topological Hall effects in charge and heat transport. Low critical currents needed to manipulate skyrmions opened a new active field of research – skyrmionics, which has a goal of developing skyrmion-based magnetic memory and data processing devices. I will discuss skyrmions and half-skyrmions in magnets with competing exchange interactions, in particular, their dynamic and multiferroic properties that make possible to control these topological defects with an applied electric field.

Material development and nanostructure optimization for devices based on thermoelectric and thermomagnetic phenomena

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Thermoelectric conversion efficiency is intrinsically limited due to interdependence of the thermal and electrical conductivity of the materials employed. Recently, a spin-based approach has been discovered and in analogy named the spin Seebeck effect (SSE)[1]. The SSE refers to the generation of spin currents in a magnetic material upon application of a temperature gradient; the spin current is injected and electrically detected in a normal metal in contact with magnetic material, where spin-orbit interaction in normal metal transforms the spin current into an electric field, by means of the inverse spin Hall Effect.

The observation of the Spin Seebeck Effect (SSE) in magnetic insulators has opened the possibility to generate pure spin currents with less dissipation losses due absence of mobile charge carriers, and further expand the range of possible materials to study spin mediated thermoelectric conversion. Moreover, the experimental geometry of the SSE with the thermal and electric current paths perpendicular to each other is advantageous for the implementation of thin film and flexible thermoelectric devices [2]. Furthermore, since the heat and electric currents have independent paths, the properties of different materials comprising the SSE hybrid device can be optimized independently. However, there is one main disadvantage for the potential application of the SSE, the low magnitude of the thermoelectric output. Different possibilities are currently being explored, such as increasing the spin current detection efficiency by taking advantage of the spin Hall angle characteristics of different materials [3]. Other approaches can be directed towards increasing the thermal spin current generations, as recently shown in spin induced thermoelectric measurements in [Pt/Fe3O4] × n films multilayers, topic that will be described in this work [4]. A short review of advances on Spin Seebeck as well as spin Peltier Effect (SPE) [5] will be presented.

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[3] K. Uchida, H. Adachi, T. Kikkawa, A. Kirihara, M. Ishida, S. Yorozu, S. Maekawa, and E. Saitoh, Proceedings of the IEEE (2016).

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HTc superconductor-based devices: low consumption-high performance applications

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The discovery of high temperature superconductors (HTSC) in 1986 has opened prospects of widespread application of superconductors in electronics. But the transfer of this technology to industry has been retarded principally by the fact that they must be cooled to low temperatures to become superconducting. Recent advances in cryogenics have boosted HTSC devices development [1]. In this talk, we will see some examples of HTSC devices for applications in telecommunication, neuromorphic treatment of signals [2], and magnetic resonance imaging systems [3] elaborated at the Unité Mixte de Physique CNRS/Thales.

[1] European contract H2020-MSCA-RISE-2016 N° 734187 — SPICOLOST
[2] Patent WO 2014/086990 A1 « Dispositif hybride à résistance variable par commande analogique non-volatile » - J. Briatico, J.E. Villegas and R. Bernard
[3] M. Geahel, I. Jouanny, D. Gorse−Pomonti, M. Poirier−Quinot, J. Briatico, C. − J. van der Beek Edge Contamination, Bulk Disorder, Flux Front Roughening, and Multiscaling in Type II Superconducting Thin Films. Condensed Matter. 2, 27 (2017)

Regular Talk Abstracts

Dr. Néstor Ghenzi - CNEA - Buenos Aires - Argentina
"1T1R Analysis based on Load Lines”

Dr. Diego Rubi - CNEA - Buenos Aires - Argentina
"A memristive diode with giant memcapacitance"

Lic. Mercedes Linares Moreau CNEA – Buenos Aires- Argentina
“Understanding and Controlling the Local Electrical Properties of Ag and Au NP-loaded Mesoporous Titania Films by Scanning Probe Microscopy”

Dr. David Comedi - Univ. Nacional de Tucumán – Argentina
"Wide bandgap semiconductor oxide nanostructures for chemical sensing, transparent electronics and UV optoelectronics"

Dr. Mariano Quintero - CNEA - Buenos Aires - Argentina
"Magnetic entropy change in phase separated manganites"

Dr. Marcelo Stachiotti - Instituto de Física de Rosario – Argentina
"Single phase multiferroic compounds by doping ferroelectrics with magnetic ions"

Dr. Raúl Carbonio - INSTITUTO DE INVESTIGACIONES EN FISICO- QUIMICA - Córdoba- Argentina
"Perovskites, model systems for the development of multifunctional oxides: the importance of spin reorientation"

Dr. Verónica Vildosola - CNEA - Buenos Aires - Argentina
"In the search of new 2D electron systems at the surface of BaBiO3 thin films”

Lic. Santiago Carreira - CNEA – Buenos Aires- Argentina
“Tuning the Interfacial Charge, Orbital and Spin Polarization Properties in $La_{0.67}Sr_{0.33}MnO_3$/ $La_{1-x}Sr_xMnO_3$ Bilayers and Magnetic Tunnel Junctions”

Dr. N. E. Massa - Lanais EFO-Cequinor and UNLP - La Plata – Argentina
“Terahertz Spin Wave Resonances and Crystal Field Transitions in $RCrO_3$ (R=Pr, Sm, Er) at Ultra Low Temperatures”

Dr. Joaquín Sacanell - CNEA – Buenos Aires- Argentina
“Paths towards stability in PS manganites: aging/rejuvenation and thermal training effects”

Dr. Rodolfo Fuentes - CNEA – Buenos Aires- Argentina

“Nanostructured Pd/lanthanide doped ceria oxides with high catalytic activity for CH4 combustion”

Dr. Gabriela Leyva - CNEA – Buenos Aires- Argentina
“Synthesis of nanostructured mixed oxides, morphology and properties”

1T1R Analysis based on Load Lines

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The electrical response of one thin-film transistor (1T) plus one resistive switching (1R) memory device in the same structure (1T1R) was characterized. The thin-film transistor (TFT) is based on an amorphous inorganic semiconductor layer deposited on a high-*k* dielectric (acting as gate dielectric). The active layer of the resistive switching (RS) device is also fabricated with a binary oxide. When the deposition parameters of the semiconducting channel layer and the gate dielectric of the TFT, and those of the active layer of the RS device are changed, the individual response of these components is strongly affected. This requires an adjustment of the geometrical characteristic of the TFT, that is, the W/L ratio. Through the load line analysis, the optimum deposition and electrical operation conditions to obtain maximum RS amplitude were determined, as well as the minimum W/L to minimize the total area of the TFT.

The integration of RS devices in large-area electronic circuits presents two potential advantages. First, it incorporates useful functionalities in trivially simple devices; the clearest example is that one can have a multilevel non-volatile memory with just a simple structure. Many other functionalities have being reported, ranging from reconfigurable rectifier and light-sensitive switch to logical implication and bio-inspired functions [5]. In the other hand, RS fabrication steps, in general, are well compatible with large-area electronics processes. Nevertheless, large-area electronics circuits are based on TFT whose typical field-effect mobilities are below 10 cm^2/Vs. Therefore, the circuit to command the RS device has to deal with limited available current in first place, and then, with an ON resistance of the TFT channel comparable with the resistance of the RS device. In this talk, the analysis of the load lines in TFT response to determine the optimal deposition conditions and to find the minimum W/L value is explained. This analysis method is validated in 1T1R configurations based on inorganic TFTs and redox-based RS devices.

A memristive diode with giant memcapacitance

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Resistive switching (RS) is defined as the reversible and non-volatile change of the electrical resistance of metal-insulator-metal structures upon the application of electrical stress [1]. This effect may lead to the development of a new generation of micro and nano-electronics devices, such as non-volatile (RRAM) memories and disruptive devices presenting neuromorphic behavior.

RS has been ubiquitously found in transition metal oxides, including complex oxides usually known as manganites. Several RS mechanisms have been proposed, and usually different mechanisms can coexist in single systems [2]. Here we address the RS behavior found on epitaxial thin films of the manganite $La_{0.5}Sr_{0.5}Mn_{0.5}Co_{0.5}O_{3-\delta}$ (LSMCO) grown on Nb:$SrTiO_3$ substrates. This manganite has the particularity of presenting two stable phases with a significant difference in their oxygen stochiometry [3] and resistivity. We show that it is possible to switch between both phases by the application of external electrical stress. Based on thorough electrical characterization, we show that RS takes place at the manganite/substrate interface, where a switchable *p-n* diode is formed. In addition, we found that the RS process is concomitant with a giant memcapacitance effect, which opens interesting possibilities for RF applications.

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Understanding and Controlling the Local Electrical Properties of Ag and Au NP-loaded Mesoporous Titania Films by Scanning Probe Microscopy

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Mesoporous titania (MT) thin films present a variety of applications in several fields, such as catalysis, optics, sensing and biomaterials, among others. Loading MT with metallic nanoparticles (NPs) inside the pores allows to take advantage of the size and confinement of the NPs, protecting them from the environment [1,2]. In this work we present a study of the local effects in the electrical properties and topography of MT thin films embedded with gold and silver NPs, by means of different Scanning Probe Microscopy techniques. These studies are relevant in the development and characterization of micro- and nanodevices based on TiO_2 and TiO_2-metal nanocomposites.

The MT films were synthesized by sol-gel and dip coating, using conductive Si substrates. Metallic NPs were incorporated to the films using two methods: stepwise reduction of $AuCl_4^-$ with $NaBH_4$ for the MT-Au samples [3]; and photoreduction of Ag^+ in solution for the MT-Ag samples [4]. Sample morphology was studied by SEM and spectroscopic ellipsometry. Local electrical transport was studied by Conducting Atomic Force Microscopy (CAFM), contact surface potential by Kelvin Probe Force Microscopy (KPFM) and local capacitance contrast by Scanning Capacitance Microscopy (SCM).

Using these SPM techniques we were able to correlate the local electrical properties with the morphology of the samples. For the MT-Au case, KPFM and SCM measurements provided information on the distribution of the Au NPs inside the film even when they are not electrically ‘connected’ to the substrate, in contrast to CAFM images. Under certain conditions we found that it is possible to locally modify the electric resistance and topography using CAFM scans with bias voltage for both systems. These results were compared to previous studies in the MT film with no NPs, in which we have confirmed a similar effect that depends strongly on ambient humidity and film porosity [5].

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Wide bandgap semiconductor oxide nanostructures for chemical sensing, transparent electronics and UV optoelectronics

David Comedi

NanoProject group and LAFISO, Departamento de Física, Facultad de Ciencias Exactas y Tecnología, Universidad Nacional de Tucumán, and Instituto de Física del Noroeste Argentino - INFINOA (UNT-CONICET)

Wide bandgap oxide semiconductor oxides are multifunctional materials that are being intensively studied for their important potential applications in transparent electronics, spintronics, UV photonics, photovoltaics, UV optoelectronics, chemical sensing and many more. A giant variety of synthesis routes have followed from demands for controlling increasingly complex electronic structures, morphologies and optoelectronic properties of proposed novel nanostructures. This has been concomitant to the development of new experiments intended to elucidate the intriguing properties and effects that result both from the nanosize of the studied systems as well as from peculiarities of the mechanisms active during their growth.

In this talk, I will focus on ZnO nanowires and related materials such as ZnO/MgO core/shell structures and ZnNiO alloys. In particular, I will describe developments and results achieved by our NanoProject group in Tucumán at our recently created Physics Institute of Northwester Argentina - INFINOA (CONICET-UNT) in three of our projects: 1) the synthesis from the vapor, manipulation and functionalization of ZnO nanowires for the development of highly sensitive nanostructured enzymatic glucose biosensors; 2) the physics and chemistry of ZnO nanowire surface passivation by transparent MgO layers to yield useful core/shell encapsulated nanostructured systems towards the development of ZnO based UV-LED; and 3) the science behind the sol-gel fabrication and properties of transparent ZnNiO thin films with potential application as an active semiconductor material in transparent electronics.

Magnetic entropy change in phase separated manganites.

Mariano Quintero

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The magnetocaloric effect (MCE) is the temperature change observed in a magnetic system when an external magnetic field is applied. The main motivation for the study of this phenomenon is the potential use in refrigeration devices based in the MCE.

In that sense, manganites became one of the most promising materials for use in magnetic refrigeration. This is due to the possibility of being able to tune their magnetic properties with some ease. However, the complexity of the phase diagram of the manganites can lead to errors when determining the characteristic parameters of the MCE (typically the change of magnetic entropy).

In this paper we will focus on the aspects related to the methods to determine the entropy change following different paths. We will analyze how the results change depending on whether direct methods (such as specific heat measurement) or indirect methods are used (using Maxwell's formula).

Single phase multiferroic compounds by doping ferroelectrics with magnetic ions

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In this talk I present the effects of Fe doping on electric and magnetic properties of two ferroelectric oxides: $Bi_4Ti_3O_{12}$ (BIT) and $PbZr_{0.52}Ti_{0.48}O_3$ (PZT). BIT is one of the simplest compounds in the Aurivillius family with a vast potential for applications, specially as NvRAMs. PZT is the dominant ferroelectric material for practical applications because of its large piezoelectric constant and large remnant polarization. To ensure charge neutrality, the strategy is to develop multiferroics from those oxides by Fe^{3+}/Nb^{5+} co-substitution on $(Ti\text{-}Zr)^{4+}$ sites. For that purpose, $Bi_4Ti_{3-x}(Nb_{0.5}Fe_{0.5})_xO_{12}$ ceramics were synthesized and we show that the structure for the compounds with $x \leq 1$ is the characteristic one of the n=3 member of the Aurivillius family. Raman measurements corroborated that both Fe^{3+} and Nb^{5+} ions are incorporated into the Ti sites. Dielectric studies at room-temperature displayed the reduction of dielectric constant and loss tangent with substitution, while the switching behavior shows ferroelectric character. Magnetic measurements indicated antiferromagnetic spin correlations between Fe^{3+} ions. The results are corroborated by first-principles calculations on $Bi_4TiNbFeO_{12}$, which predict an electric polarization of ~30uC/cm^2 and confirm the antiferromagnetic ground state, for which we obtain a nearest-neighbor super-exchange coupling J=7meV. We assessed different B sites configurations and found a preference for Fe^{3+} ions to be located at the outer perovskite B sites. For the case of PZT, $[PbFe_{0.5}Nb_{0.5}O_3]_{0.5}$ $[PbZr_{0.52}Ti_{0.48}O_3]_{0.5}$ thin films were fabricated by a chemical solution deposition technique. The films were prepared by spin-coating on $Pt/TiO_x/SiO_2/Si$ substrates and thermally treated by rapid thermal annealing. We observed the coexistence of ferroelectric and ferromagnetic properties at room temperature, similar to what was reported in bulk ceramics.

Perovskytes, model systems for the development of multifunctional oxides: the importance of spin reorientation

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Perovskyte oxides are known to have multiferroic [1], magnetoelectric [2], magnetodielectric [3, 4] and magnetocaloric [5] properties. It has been shown that there are some correlations between some of these properties and spin reorientation (SR) phenomena [1-6]. Particularly, for $SmFeO_3$ the presence of significant anomalies in the temperature dependent dielectric behavior across spin reorientation transition temperature indicate magneto electrical coupling [6].

Based on these findings, we start a systematic study of spin reorientation in $RFe_{0.5}Cr_{0.5}O_3$ perovskites (R= Tb, Dy, Ho, Er, Tm, Yb, Lu) using magnetization measurements as a function of T and H and powder neutron diffraction (PND). In general a progressive transition from a G_4 to G_2 spin configuration of the transition metal sublattice is observed as temperature is lowered for most of the compounds. For the diamagnetic Lu^{3+} compound no SR is observed which shows that the magnetic mean field generated by the paramagnetic lanthanide is responsible for the SR phenomena.

I will present in this conference a brief SR phenomena analysis using the PND data and in some cases correlations found between magnetodielectric properties and SR transition.

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In the search of new 2D electron systems at the surface of BaBiO3 thin films

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The presence of 2D electron systems (2DES) at surfaces or interfaces in oxide thin films remains a hot topic in condensed matter physics. In particular, BaBiO3 is a material with fascinating properties already in bulk, presenting a charge ordered insulating phase that is in proximity of a superconducting one upon doping. It has also been suggested as a topological material very recently. In a previous work, we have theoretically proposed that its (001) surface should become metallic if a Bi-termination is achieved and the mechanism behind this effect is predicted to be independent of the presence of oxygen vacancies or polar discontinuities. Here we report on the preparation by pulsed laser deposition and characterization of BaBiO3 thin films on silicon. We show that the texture of the films can be tuned by controlling the growth conditions, being possible to stabilize strongly (100)-textured films. We find significant differences on the spectroscopic and transport properties between (100)-textured and non-textured films. We rationalize these experimental results by performing first principles calculations, which indicate the existence of electron doping at the (100) surface. This stabilizes Bi ions in a 3+ state, shortens Bi-O bonds and reduces the electronic band gap, increasing the surface conductivity. Our results emphasize the importance of surface effects on the electronic properties of perovskites, and provide strategies to design novel oxide heterostructures with potential interface-related 2DES.

Tuning the Interfacial Charge, Orbital and Spin Polarization Properties in $La_{0.67}Sr_{0.33}MnO_3$/ $La_{1-x}Sr_xMnO_3$ Bilayers and Magnetic Tunnel Junctions

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The possibility of studying and controlling oxide interfaces is still intriguing researchers owing to their potential applications in spintronic devices among other technologies. The case of $La_{0.7}Sr_{0.3}MnO_3$ ($LS_{0.3}MO$) is particularly interesting, as it is ferromagnetic with a high Curie temperature (Tc ~ 370 K) and has a half-metallic character. However, the tunneling magnetoresistance (TMR) ratios obtained in magnetic tunnel junctions made with this manganite are much smaller than expected.[1] The reduction of the spin polarization at the interface has been usually attributed to surface symmetry breaking effects, preferential orbital occupation, strain and charge transfer.[2,3] Here, we present synchrotron studies of $LS_xMO/LS_{0.3}MO$ bilayers grown by pulsed laser deposition on $SrTiO_3(001)$ substrates, where the tunnel barriers are low doped manganites with Sr doping $0 \leq x \leq 0.1$ and 2 - 6 nm thick. By combining surface sensitive techniques such as XAS, XMCD and XLD, we are able to describe the magnetic order, oxidation states, electronic orbital occupation and spin-polarization at interfaces. Synchrotron experiments suggest the existence of an optimal barrier thickness with the higher spin-polarization. We explain the non-trivial magnetic profile by the combined effect of two mechanisms. On one hand, the extra carriers supplied by the low-doped manganites tend to compensate the over-doped interface, favoring the existence of ferromagnetic zones where the double-exchange coupling dominates. Besides, the evolution from a tensile-strained structure of the inner layers to a compressed-structure at the surface changes gradually the orbital occupation and hybridization of the 3d-Mn orbitals, being detrimental for the spin polarization of the electronic bands. Moreover, we found clear evidence of spin polarization at the La sites, which can be driven by charge migration through the La-O hybridized orbitals. Finally, we discuss the effects of the LS_xMO on the TMR in modified tunnel junctions $LSMO/LS_xMO/STO/LS_xMO/LSMO$.

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Terahertz Spin Wave Resonances and Crystal Field Transitions in $RCrO_3$ (R=Pr, Sm, Er) at Ultra Low Temperatures

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The possibility of developing materials with magnetic order simultaneous with a polar state has given rise to great activity seeking to optimize dielectric and magnetic interactions. Of these, the distorted perovskites, orthoferrites and orthochromites, are a group of oxides in which the greatest attention has been focused due to their nominal structural simplicity and potential multiferroic properties. They are considered centrosymmetric orthorhombic compounds belonging at room temperature to the spatial group P_{bnm}-D^{2h}_{16} with four molecules per unit cell with complex exchanges due to the two magnetic ions (M =transition metal, R = rare earth) M^{3+} -M^{3+}, M^{3+} -R^{3+}, R^{3+} -R^{3+}. More recently, high-resolution diffraction patterns on $RCrO_3$ (R=Rare Earth) brought up a weak lattice distortion out of orthorhombic centrosymmetric that might have strong implications when weighing the Moriya spin-orbit coupling, and the associated Dzyaloshinkii field (DM interaction) against symmetric exchange. Overall, the transition metal sublattice turn antiferromagnetic below T_N in the Γ_4 (G_x, A_y, F_z) irreducible representation. It also develops distinctive weak ferromagnetism (F_z) originating in spin canting of the M^{3+} moment relative to the plane ***ab***. The spontaneous magnetization of the transition metal , being antiparallel to the moment of the rare earth, changes at T_{SR} of oriented along the axis ***a*** to parallel to the axis ***c.***The equations of motion of the two magnetization sublattices of the transition metal are linked by the exchange interaction describe different precessions. They give rise to two resonant modes that exist due to exchange fields and anisotropies. The optical detection of these spin resonances arise when the magnetic field ***H*** of the THz radiation couples to spin oscillations.

Here we present absorption measurements made in HZB, BESSY II, Berlin, due to rare earth crystalline field transitions and spin wave resonant modes of the transition metal in polycrystalline isomorphic compounds $RCrO_3$ (R = Pr , Sm, Er) under magnetic fields up to 10 T and at ultra-low temperatures.

The absence of spin reorientation in $PrCrO_3$ (T_N(Cr) ~238 K), where the Pr sublattice remains paramagnetic up to at least ~1.4 K, has as consequence the non-detection of spin resonances in our range of temperatures. We found a single singlet as dominant feature in PrCrO3 (Pr is a $4f^2$ non-Kramers ion) emerging at ~39 cm^{-1} and ~100 K that in consonance with emerging new infrared active phonons suggests a gradual change in the network

associated to the polar character of the antiferromagnetic phase. Under external magnetic fields H_0 the Zeeman split has a linear behavior turning quadratic which deviates above ~7 T likely due to structural deformations induced by the stronger field. Contrary to this, $SmCrO_3$ (T_N (Cr) ~97 K) has no detectable crystal field transitions, probably, due to the near canceling of the spin and orbital moments as found for isomorphs $SmCoO_3$ in the $^6H_{5/2}$ multiplet (L=5, S=5/2, J=L – S=5/2) at temperatures below T_{SR} <40 K. This facilitates detection of the temperature dependent AFM and FM spin wave resonances. At lower applied magnetic field they have a linear splitting that increasing H_0 turn both band profiles bands into weak broad contours. In $ErCrO_3$ (T_N (Cr) ~133 K) the crystalline field transitions as well as a weaker one attributed to AFM appear at T_{SR} <22 K suggesting that the reorientation of spins is accompanied by a structural change. The Kramers doublet of Er $4f^{11}$ configuration unfolds clearly. Each component is additionally Zeeman split by the external magnetic field and remarkably, there is a further split in the higher energy branch at fields strong enough to induce ferromagnetism by spin reorientation. Increasing fields the AFM and FM modes merge into a continuum suggesting an environment of magnetic and electric dipoles globally entangled in the unstable framework of the already volatile perovskite lattice.

Taken together, our measurements suggest a detail not foreseen by the existing literature but that should be taken into account when recreating the properties of these compounds.

PATHS TOWARDS STABILITY IN PS MANGANITES: AGING/REJUVENATION AND THERMAL TRAINING EFFECTS

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In this work we address the interplay between two phenomena which are signatures of the out-of-equilibrium state in phase separated (PS) manganites: irreversibility against thermal cycling and aging/rejuvenation process. The sample investigated is $La_{0.5}Ca_{0.5}MnO_3$, a prototypical manganite exhibiting phase separation. Two regimes for isothermal relaxation were observed according to the temperature range: for T > 100 K, aging/rejuvenation effects are observed, while for T < 100 K an irreversible aging was found. Our results show that thermal cycles act as a tool to unveil the dynamical behavior of the PS state in manganites, reveling the close interplay between static and dynamic properties of phase separated manganites.

Nanostructured Pd/lanthanide-doped ceria oxides with high catalytic activity for CH_4 combustion

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Ceria-based mixed oxides are materials with a large technological impact, especially in the area of environmental protection. Nanostructured ceria materials can be used as supports for highly dispersed noble metal nanoparticles. The resulting catalyst systems exhibit much improved catalytic activity and redox properties. In particular, Pd-based catalysts are active for NO reduction and CO and hydrocarbon oxidation reactions. Enhanced metal-support interactions led to exceptionally high methane oxidation, with complete conversion below 400 °C. [1]

In this work, nanostructured $Ce_{0.9}Ln_{0.1}O_{2-d}$ (LnDC; Ln: Gd, Pr, Tb) spheres previously obtained by microwave assisted hydrothermal homogeneous co-precipitation (HMW)[2,3] were impregnated with 1% wt Pd by incipient wetness impregnation (WI) of an aqueous Pd2+ solution. Their properties were characterized by synchrotron radiation X-ray diffraction (SR-XRD), X-ray absorption near-edge spectroscopy (XANES) and scanning and high resolution electron microscopy (SEM and HRTEM) with X-ray spectroscopy (EDS). In situ XRD and XANES experiments were carried out under reducing and oxidizing conditions in order to investigate the redox behaviour of these materials. The addition of Pd to the LnDC increased the reducibility of the Ce in the mixed oxide. This was demonstrated by analysis of in situ XANES spectra obtained under reducing conditions. Clearly, the Pd improves the Ce^{3+}/C^{e4+} redox couple in LnDC materials. High activity for CH_4 oxidation was observed in nanostructrured Pd/LnDC spheres with a total conversion of CH_4 temperature lower than 400 ºC. In fact, the reaction rates here reported at 350 ºC show the highest efficiency per palladium atom in comparison with other palladium-based catalysts reported in literature.[1,4] These findings open up an interesting avenue for future working this area, and indicate a promising possible application for this particular system.

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Synthesis of nanostructured mixed oxides, morphology and properties

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Nanostructured mixed oxides show interesting properties for technological applications. In particular, different mixed oxides with perovskite structure and doped ceria with cubic crystalline structure were studied. These materials present catalytic properties and can be used in heterogeneous phase reactions or as electrodes for solid oxides fuel cells.

The synthesis method plays an important role in the morphology and can modify the properties of the products. We explore the synthesis of nanostructured wires and tubes using a template method and nanoparticles through a hydrothermal co-precipitation method assisted by microwaves.

POSTERS

Annealing influence on Germanium MOSCAPs: Degradation

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Forming gas annealing Influence (FGA) on nano-laminated Ge based MOS capacitors is analyzed by the C-V hysteresis and flat band voltage shifts for negative and positive stress fields. We found that the FGA (H_2/N_2) treatment does not affect the electron trapping observed at positive stress bias, while it reduces the positive charge trapping in high-K/Ge stacks for stress at negative bias, which is a common trend regardless of the $Al_2O_3/HfMO_x$ stack. It indicates that a considerable part of the interface defects with energies close to the valence band existing in the oxide-semiconductor interface result passivated during the FGA. Considering the results in terms of the integration with III-V materials, Ge-and InGaAs-based MOS stacks show opposite dependencies on the FGA process.

Performance optimization of vapour sensors based on porous photonic crystals and Tamm plasmons

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The design and construction of one-dimensional porous photonic crystals (PCs) and Tamm plasmon based sensors are presented in this work. PCs are multi-layered materials with a periodic modulation of the layers refractive index on a scale comparable to the wavelength of visible light, which gives them intense colours due to reflection.[1] These materials can be modified with a thin layer of a noble metal, to give rise to a new type of sensors based on the Tamm plasmon resonance.[2,3]

The PCs were synthesized by alternated deposition of titanium and silicon oxides with controlled porosity. For the Tamm sensor construction, a gold thin film was deposited over the highest refractive index layer (TiO2) of the PCs2. The gold layer was then protected with a very thin porous titania film, to obtain a more robust device. This protective layer does not affect significantly the device optical and sensing properties.

The devices were evaluated as sensors for several organic vapours by measuring the variation of the maximum specular reflectivity of the stop band for the PCs or the Tamm mode. It was found that the Tamm plasmon based sensors present higher sensibility and Figure of Merit than the PCs, making them promising platforms for the development of different kind of vapours and liquids sensors.

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STRUCTURAL FASES AT REDUCED CeO_2 (111) SURFACES

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The singular ability of ceria (CeO_2) to release and store oxygen is extensively exploited in catalysis and other applications such as fuel cells, sensors and non-volatile memories. The knowledge and control of the ordering of oxygen vacancies and charges is fundamental to develop and optimize the ceria functionality in these applications. In recent works, we studied the defect structure of reduced bulk and its (111) surface [1-3] using Density Functional Theory (DFT) in its DFT+U approximation, identifying different patterns for the location of vacancies and charges, and explaining the formation of experimentally observed structures.

In this work, we investigate the reconstructions of the CeO_2(111) surface that occur as the temperature increases upon annealing [4]. Through non-contact force microscopy (NC-AFM), we observed the consecutive formation of five different periodic structures, including a ($\sqrt{7} \times 3$) structure that was not previously reported. Using DFT+U calculations, we modeled the distribution of vacancies and Ce^{3+} cations. We show that this new ($\sqrt{7} \times 3$) structure does not correspond to a stable bulk structure and can only be stabilized as a thin surface layer. Finally, using ab initio thermodynamics, we explain the stability of the different surface phases under reducing conditions.

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Influence of thermal properties of high-k dielectrics on the dynamics of progressive breakdown in MIM structures

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In advanced MIM and MIS devices, the breakdown (BD) phenomenon, i.e. the formation of a filamentary pathway spanning the dielectric film, occurs in the regime of relatively low voltage and high electric field [1]. It is well known that this degradation process is related to the generation of a large density of electronic defects promoted by the transport of energetic carriers through the film[1, 2].When a critical density of defects is reached, a localized percolative path is formed. Beyond this point, the oxide BD evolution in very thin films is characterized by a gradual or progressive growth of the leakage current that flows through the device. Besides the relevance of these effects for the scaling of gate dielectrics of transistors in modern CMOS integrated circuits, further insight into the BD physics may also provide a reference framework for different applications of ultra-thin dielectrics, such as, for example, the electrically induced resistive switching (RS) effect. Recently, the main physical mechanism behind the progressive BD (PBD) dynamics was identified [3– 5]. The high temperature associated with the localized current flow would promote electro-migration of the fastest atomic species among those available, thus contributing to the enlargement of the BD filament. Within this framework, the thermal conductivity of the oxide layer would play a fundamental role in the PBD growth.

Additionally, it should be considered, as suggested in [6], that this effect can be linked to a gradual transfer of the dissipated power from the bottleneck of the BD path to the electrodes, which helps on explaining the sustainability of such a large current density in an atomic size filamentary path.

In this work, the influence of the oxide thermal conductivity in the PBD dynamics for the case of MIM stacks has been investigated. Since BD is strongly associated with power dissipation, the potential role played by the metal electrodes needs to be explored in MIM stacks. The use of two dielectric layers (Al_2O_3 and HfO_2) with large differences in their thermal properties ($\kappa_{Al2O3}\approx30$ W/mK; $\kappa_{HfO2}=1.1$ W/mK) allowed to qualitatively assess the influence of the oxide layer on the PBD dynamics.

Current was monitored using a high bandwidth setup until the occurrence of the fast BD event, and the characteristic rise times for different applied voltages and for both sets of samples (MIM structures with Al_2O_3 and HfO_2) were studied. The main feature of this plot

is that the rise times for Al2O3 devices are of the same order of magnitude as for HfO_2 devices, but occurring at higher applied voltages.

The capability of different insulating materials to transfer heat from the conductive filament to the bulk of the oxide, represented through their thermal conductivities, has a strong impact on the PBD dynamics in MOS structures with different material stacks. The difference of about 30 times between thermal conductivities provides the Al_2O_3 the capability to maintain the temperature of the BD path below the melting point for longer times, thus increasing the duration of the BD transient.

Additionally, lower voltage stress was performed on both types of samples, analyzing I-t characteristics of the MIM structures under different conductance states, characteristics of resistive switching devices. The results also point towards the larger times observer for Al_2O_3 when compared to HfO_2 based devices, even at very different conductance states: Al_2O_3 is able to withstand higher currents for longer times even after the forming process, i.e. with a conductive path effectively formed between the electrodes.

This leads to the idea that the thermal mechanisms that govern PBD and resistive switching strongly depend on the capabilities of the insulating layers to dissipate the heat generated along the conductive filament to its surrounding atomic network, with little, or no, influence of the electrode materials.

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Magnesium ferrite thin films: role of interface film/substrate on structural, magnetic and electric properties.

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In order to fabricate multifunctional electronic devices, researchers have focused on the study of interfacial structures between two materials with distinct symmetry groups and electronic properties. At the interfaces between oxides, electronic systems with unusual electronic properties can be generated. In this work the interface effect between Mg ferrite and single crystalline substrates (MgO or $SrTiO_3$ (STO)) is explored. Mg ferrite ($MgFe_2O_4$) thin films were grown by a Fe-O/Mg-O multilayer process using DC magnetron sputtering on MgO (100) and STO (100) substrates. The samples show high values of saturation magnetization and Curie temperatures above room temperature. While in the case of the sample grown on MgO the hysteresis loops indicate the existence of more than one ferrimagnetic component and lower value of remanence to saturation ratio, the deposited one on STO is mono-component and has a rectangular-shape magnetic loop at alltemperatures below 300 K. The difference is attributed to different microstructures due to the misfit strain caused by the different lattice constants between substrates and ferrite. The electric transport and photoconductivity properties have been investigated on both samples indicating the important role of the STO substrate in the generation of photo carriers and on the final properties of the $MgFe_2O_4$ thin films.

Rhombohedral *R3c* to orthorhombic *Pnma* phase transition induced by Y-doping in $BiFeO_3$

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In this work we study, by means of *ab initio* calculations, the structural, electronic and magnetic properties of the Y-doped $BiFeO_3$ compounds. We determine that there is a morphotropic phase boundary at an yttrium concentration of 19%, where the structure changes from an *R3c* to a *Pnma* symmetry. This structural transition is driven by chemical pressure induced by the dopant.

By analyzing the evolution of the oxygen octahedral tilts we find an enhanced antiferrodistortive distortion when increasing the Y-doping, together with a reduction of the ferroelectric distorsion, giving a lower value of the electric polarization. These cooperative effects might lead to a larger canting of the Fe magnetic moments and to a larger ferromagnetic response in the *R3c* phase, observed in the experiments.