VIII Reunión Grupo Especializado de Física del Estado Sólido

Programa definitivo y libro de resúmenes

Comité organizador:

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Las anteriores reuniones del Grupo Especializado de Física del Estado Sólido de la Real Sociedad Española de Física, celebradas en Madrid (2000), Calella (2002), San Sebastián (2004), Alicante (2006), Santiago de Compostela (2008), Zaragoza (2010) y Sevilla (2012) fueron un foro de discusión y presentación de los temas más actuales en Física de Estado Sólido tanto a nivel nacional como internacional.

En la reunión de Ciudad Real hemos pretendido mantener el mismo espíritu. Pensamos que el programa es muy atractivo, con charlas invitadas de gran calidad, interés y actualidad, y contribuciones orales y de tipo póster de muy buen nivel.

La reunión tendrá lugar en el paraninfo del Rectorado de la Universidad de Castilla-La Mancha, en el edificio de la Real Casa de la Misericordia. Como habréis podido comprobar, todos los hoteles, servicios de transporte (AVE) y restauración se encuentran a muy corta distancia de la sede del congreso.

Os agradecemos a todos vuestra contribución a esta reunión GEFES 2014, y esperamos que disfrutéis de la misma

El Comité Organizador

PROGRAMA

	Miércoles 22	Jueves 23	Viernes 24
08:00-09:00	Entrega de documentación		
09:00-09:15	Inauguración		
09:15-10:00	Invitada 1 **Francisco Guinea** ICMM-CSIC, Madrid **"Elastic properties of graphene"**	Invitada 3 **Gerrit Bauer** Tohoku University, Sendai **"Spin caloritronics – more than spin-dependent thermoelectrics"**	Invitada 5 **Jacqueline Bloch** LPN/CNRS, Marcoussis, France **"Polariton condensates in photonic circuits"**
10:00-10:20	S1-Oral invitada: Pablo Alonso-González (CICnanoGUNE, Donostia) Optical nano-imaging of gate-tuneable graphene plasmons	S3-Oral invitada: A. Carretero-Genevrier (CNRS, Lyon) Integrating functional oxide nanomaterials in silicon technology by chemical solution deposition	S5-Oral invitada: Elena del Valle (UAM, Madrid) Engineering quantum light sources through frequency filtering
10:20-10:40	S1-Oral invitada: Andrés Castellanos-Gómez (TU Delft) Nanomechanics and strain engineering in atomically thin MoS_2	S3-Oral invitada: L. Martínez (ICMM-CSIC, Madrid) Tailoring nanoparticles: controlled size, composition and structure in a one-step process	S5-Oral invitada: Pablo Molina (UAM, Madrid) Enhancement of the nonlinear response and the spontaneous emission of Nd3+ doped $LiNbO_3$ by silver nanoparticles arrays
10:40-11:00	S1-Oral invitada: Lucas Pérez (UCM, Madrid) Looking for quantum size effects in bismuth thin films and nanowires	S3-Oral invitada: Andréu Cabot (ICREA, Barcelona) Solution processing of energy conversion materials and devices: photovoltaics and thermoelectrics	S5-Oral invitada: Vanda Godinho (ICMS-CSIC, Univ. de Sevilla) New bottom-up methodology to produce silicon layers with a closed porosity nanostructure and reduced refractive index
11:05-11:35	Pausa café	Pausa café	Pausa café
11:35-12:20	Invitada 2 **Bernhard Keimer** Max Planck Institute, Stuttgart **"Control of collective quantum phenomena in metal-oxide superlattices"**	Invitada 4 **Sebastian Loth** Max Planck Institute, Darmstadt **"Magnetism at the single atom level"**	11:40 S5-Oral: Mario Culebras (Univ. Valencia) Semiconducting polymers with a high figure of merit 12:00 S5-Oral: Fabrice Laussy (UAM, Madrid) Propagation of polariton waves and polariton wavepackets
12:20-12:40	S1-Oral: Carlos Sabater (K-Onnes Lab., Leiden) Experimental evidence for Topological Insulator behaviour in atomic layers of Bismuth (111) at room temperature	S3-Oral invitada: Rocío Ranchal (UCM, Madrid) Tuning the magnetic domain patterns of sputtered TbFeGa alloys	12:20-13:40 Premios pósters y clausura
12:40-13:00	S1-Oral: Verónica León (UCLM, Ciudad Real) Graphene derivatives from Ball-milling of graphite	S3-Oral: Óscar J. Durá (UCLM, Ciudad Real) Grain boundary effect on ionic transport in yttria stabilized zirconia	
13:00-13:20	S1-Oral: Á. Gómez-León (ICMM-CSIC) Floquet-Bloch theory, irradiated graphene and topological phases	S3-Oral: Ignasi Fina (Max Planck Institute-ICMAB-CSIC) Different routes for enhanced control of ferroelectric polarization by magnetic field	
13.20-13:40	S1-Oral: José Luis Valverde (UCLM Ciudad Real- Graphenano) Carbon nanostructures: application perspectives from the commercial point of view.	S3-Oral: J. Tornos (UCM, Madrid) Ferroelectric control of spin transport in oxide magnetic tunnel junctions	

	Miércoles 22	Jueves 23	Viernes 24
13:40-15:20	Comida-Lunch	Comida-Lunch	13:40 Vino de despedida
15:20-15:40	S2-Oral invitada: José I. Martínez ICMM-CSIC, Madrid Theoretical STM Characterization of Organics on Surfaces	S4-Oral invitada: J. Herrero-Martín (ALBA Sync. Light Source, Barcelona) Intersite charge transfer and spin state transitions in Pr-based cobalt oxides by x-ray absorption/emission spectroscopies	**Sesiones:** S1- Grafeno y otros sistemas de baja dimensionalidad. S2- Propiedades físicas de sólidos en la nanoescala, física de superficies e intercaras, microscopías de proximidad y microscopía electrónica. S3- Materiales funcionales con aplicaciones en espintrónica, caloritrónica y energía. S4- Magnetismo, superconductividad, información cuántica, electrónica y magnetismo molecular, materiales complejos. S5- Propiedades ópticas, materiales y dispositivos fotónicos, semiconductores.
15:40-16:00	S2-Oral invitada: Dimas G. de Oteyza Univ. of California,Berkeley Direct Imaging of Covalent Bond Structure in Single-Molecule Chemical Reactions	S4-Oral invitada: Imanol de Pedro(Univ. de Cantabria, Santander) Magnetic properties of ionic liquids exhibiting three-dimensional magnetic order in their condensed phases	
16:00-16:20	S2-Oral: Verónica Salgueiriño(CACTI-Univ. de Vigo) Exchange Bias Effect in CoO@Fe3O4 core-shell octahedron-shaped nanoparticles	S4-Oral invitada: I. Guillamón (HH Wills Physics Lab, Bristol/UAM, Madrid) Damping of quantum oscillations in the superconducting state of MgB_2	
16:20-16:40	S2-Oral: Beatriz Rivas-Murias (CIQUS-Univ. de Santiago) Strain-induced ferromagnetism in $LaCoO_3$ and interface coupling in magnetic multilayers	S4-Oral invitada: Belén Paredes (Inst. de Física Teórica- CSIC/UAM, Madrid) Quantum merging: a physical mechanism for non-Abelian quantum matter	
16:40-17:00	S2-Oral: Milica Todorović (UAM, Madrid) Contrast Mechanisms on a Metal-Oxide Surface: Towards Chemically Selective Imaging by Controlling Tip-Apex Chemistry	S4-Oral invitada: Pablo García Fernández (Univ. Cantabria, Santander) Electrostatic control of the d_{x2-y2}-d_{3z2-r2} gap and orbital ordering in non-cubic crystals	
17:00-17:20	S2-Oral: R. Galcerán ICMAB/CSIC Tunneling magnetoresistance in Fe/MgO/La0.7Sr0.3MnO3 magnetic tunnel junctions	S4-Oral: J. Á. de Toro (UCLM Ciudad Real) A model superspin-glass: random-close-packed maghemite nanoparticles	
17:20-17:40	S2-Oral: S. Vélez (CICnanoGUNE, San Sebastián) High performance MoS_2 Field-Effect Transistors in a simple design	S4-Oral: Ricardo Zarzuela (Univ. de Barcelona) Quantum Forces in Solids	
17:40-19:20	Café + Pósters	17:40-18:00 S4-Oral: Reyes Calvo (Univ-College London) "Control of single-spin magnetic anisotropy by exchange coupling" 18:00-19:20 Café + Pósters	
21:00		Cena de gala	

CONFERENCIAS INVITADAS

Miércoles 22 de enero, 9:15 h

Elastic properties of graphene

F. Guinea

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Graphene is usually described as one of the stiffest materials known, with a Young modulus higher than steel and comparable to diamond. On the other hand, graphene is a two dimensional metallic membrane, so that strong anharmonic effects can be expected, and the electronic degrees of freedom can modify the elastic properties. These features, unique to graphene, lead to a variety of new phenomena, including a significant dependence of the elastic properties on the experimental setup used to measure them.

Miércoles 22 de enero, 11:35 h

Control of collective quantum phenomena in metal-oxide superlattices

Bernhard Keimer

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A grand challenge in the field of correlated-electron physics is the transition from conceptual understanding of collective ordering phenomena to their control and design. We will outline the first results of an experimental program designed to meet this challenge through the synthesis and characterization of metal-oxide superlattices, with particular emphasis on nickel oxides. We will show how the phase behavior of correlated electrons in these structures can be controlled by modifying the occupation of transition metal d-orbitals [1,2], the dimensionality of the electron system [3,4], and the electron-phonon interaction [5,6]. We will also show how spectroscopic methods such as resonant x-ray scattering [1,2,4], spectral ellipsometry [3], and Raman scattering [5] can be combined to obtain a comprehensive description of the electron system in metal-oxide superlattices.

[1] E. Benckiser, M. W. Haverkort, S. Brück, E. Goering, S. Macke, A. Frañó, X. Yang, O. K. Andersen, G. Cristiani, H. U. Habermeier, A. V. Boris, I. Zegkinoglou, P. Wochner, H. J. Kim, V. Hinkov, B. Keimer, Nature Materials 10, 189 (2011).
[2] M. Wu, E. Benckiser, M. W. Haverkort, A. Frano, Y. Lu, N. Nwanko, S. Brück, P. Audehm, E. Goering, S. Mache, V. Hinkov, P. Wochner, G. Christiani, S. Heinze, G. Logvenov, H.-U. Habermeier, B. Keimer, Phys. Rev. B 88, 125124 (2013).
[3] A. V. Boris, Y. Matiks, E. Benckiser, A. Frano, P. Popovich, V. Hinkov, P. Wochner, M. Castro-Colin, E. Detemple, V. K. Malik, C. Bernhard, T. Prokscha, A. Suter, Z. Salman, E. Morenzoni, G. Cristiani, H.-U. Habermeier, B. Keimer,Science 332, 937 (2011).
[4] A. Frano, E. Schierle, M. W. Haverkort, Y. Lu, M. Wu, S. Blanco-Canosa, U. Nwankwo, A. V. Boris, P. Wochner, G. Cristiani, H. U. Habermeier, G. Logvenov, V. Hinkov, E. Benckiser, E. Weschke, B. Keimer, Phys. Rev. Lett. 111, 106804 (2013).
[5] N. Driza, S. Blanco-Canosa, M. Bakr, S. Soltan, M. Khalid, L. Mustafa, K. Kawashima, G. Christiani, H.-U. Habermeier, G. Khaliullin, C. Ulrich, M. Le Tacon, B. Keimer, Nature Materials 11, 675 (2012).
[6] S. Heinze, H.-U. Habermeier, G. Cristiani, S. Blanco Canosa, M. Le Tacon, B. Keimer, Appl. Phys. Lett. 101, 131603 (2012).

Jueves 23 de enero, 9:15 h

Spin caloritronics – more than spin-dependent thermoelectrics

Gerrit E.W. Bauer[1,2]

[1] *Institute of Materials Research and WPI-AIMR, Tohoku University, Japan*
[2] *Kavli Institute of NanoScience, TU Delft, The Netherlands*

The spin degree of freedom of the electron affects not only charge, but also heat and thermoelectric transport, leading to new effects in small structures that are studied in the field of spin caloritronics (from calor, the Latin word for heat).

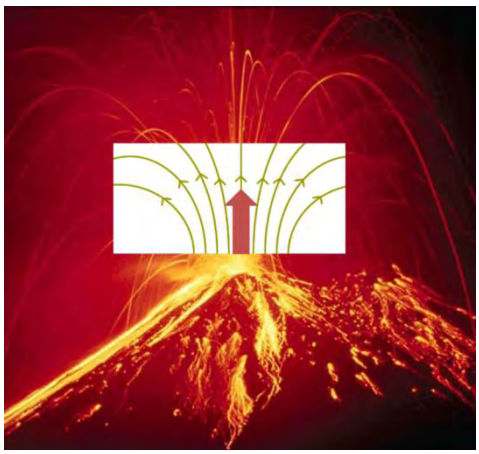
This lecture addresses the basic physics of spin caloritronics. Starting with an introduction into thermoelectrics and Onsager's reciprocity relations, the generalization to include the spin dependence in the presence of metallic ferromagnets will be addressed. Using this foundation I will describe several recently discovered spin-dependent effects in metallic nanostructures and tunneling junctions in terms of a two spin-current model of non-interacting electrons.

Next, I will argue that a different class of spin caloritronic effects exists that can be explained only by the collective spin dynamics in ferromagnets. The thermal spin transfer torque that allows excitation and switching of the magnetization in spin valves as well as the operation of nanoscale heat engines is complemented by thermal spin pumping. The latter generates the so-called spin Seebeck effect, which is generated by a heat current-induced non-equilibrium of magnons at a contact between an insulating or conducting ferromagnet and a normal metal. Under these conditions a net spin current is injected or extracted from the normal metal that can be detected by the inverse spin Hall effect.

Both classes of effects can be understood in the adiabatic approximation for the magnetization dynamics and computed in terms of material-dependent electronic structures. Further issues to be addressed are the relation between electric, thermal and acoustic actuation of the magnetic order parameter, as well as the application potential of spin caloritronics.

More details and a bibliography can be found in Ref. [1].

[1] G.E.W. Bauer, E. Saitoh, and B.J. van Wees, Spin Caloritronics, Nature Materials 11, 391 (2012).



Jueves 23 de enero, 11:35 h

Magnetism at the single atom level

Sebastian Loth

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Max Planck Institute for Solid State Physics, Stuttgart, Germany
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Magnetism in nanostructured materials provides an exciting field where technology development and fundamental research meet. Often the collective magnetic behavior of a nanostructure intricately depends on the details of spin-dependent interaction between atoms on sub-nanometer length scales. This necessitates spin-sensitive probes with atomic resolution but also enables engineering of complex magnetic functionality. In this talk we will demonstrate that scanning tunneling microscopy provides a complete toolset to shape magnetism at the single atom level.

We use a low temperature scanning tunneling microscope to access transition metal atoms on surfaces and manipulate them into atomically defined nanostructures. Spin-dependent inelastic electron tunneling can then be used to determine spin magnitude and anisotropy energies with micro-electronvolt precision [1]. With this information we design nanostructures that either enhance or suppress effects such as spin correlation, delocalization, spin lifetime or magnetic tunneling. We will discuss a new approach to create bistable nanomagnets with just a few atoms providing valuable insights for size limits in future magnetic devices [2]. Quantum mechanical behavior can be enhanced by combining atoms with different spin magnitude into chains. Arrays of several nanometers length can be placed into spin-correlated singlet ground states that exhibit Kondo-type screening.

It is crucial to measure the dynamical response of a magnet to quantify magnetic stability and identify energy loss mechanisms. We make use of GHz bandwidth electronic pulse generators to implement pump probe spectroscopy in the STM. This technique measures the nanosecond-fast spin relaxation of individual atoms. The time domain information enables non-local measurements of magnetic states and sheds light onto possible pathways to controllably interact with atom-sized quantum spins [3].

[1] C.F. Hirjibehedin et al. Science 317, 1199 (2007).
[2] S. Loth, S. Baumann, C. P. Lutz, D. M. Eigler, A. J. Heinrich, Science 335, 196 (2012).
[3] S. Yan, D. J. Choi, J. Burgess, S. Loth, *in preparation*.

Viernes 24 de enero, 9:15 h

Polariton condensates in photonic circuits

Jacqueline Bloch

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At the frontier between non-linear optics and the physics of Bose Einstein condensation, semiconductor microcavities opened a new research field, both for fundamental studies of bosonic quantum fluids in a driven dissipative system, and for the development of new devices for all optical information processing.

Optical properties of semiconductor microcavities are governed by bosonic quasi-particles named cavity polaritons, which are light-matter mixed states. Cavity polaritons propagate like photons, but interact strongly with their environment via their matter component.

After a general introduction on cavity polaritons, I will review recent experimental works performed on polariton condensates confined in microstructures.

I will first show how we can generate, in one-dimensional cavities, polariton flows which propagate over macroscopic distances (mm), while preserving their spontaneous coherence. These propagation properties can be used to implement a variety of optically controlled polariton devices: the example of a non-linear resonant tunneling polariton diode will be addressed, a device very promising to reach the quantum regime of polariton blockade.

The last part of the talk will be devoted to the physics of polaritons in periodic potentials. I will discuss polariton condensation in a 1D periodic potential, the generation of a polariton condensate in the photonic analog of a Benzene molecule (a ring of six coupled micropillars), and finally the direct visualization of Dirac cones in a honeycomb lattice (the photonic analog of graphene).

These examples highlight the great potential of semiconductor cavities as a new platform to investigate the physics of interacting bosons.

References

[1] *Spontaneous formation and optical manipulation of extended polariton condensates* , E. Wertz, et al., Nat. Phys. 6, 860 (2010).
[2] *Interactions in Confined Polariton Condensates* , L. Ferrier, et al., Phys. Rev. Lett. 106, 126401 (2011).
[3] *Backscattering suppression in supersonic 1D polariton condensates* , D. Tanese, et al., Phys. Rev. Lett. 108, 036405 (2012).
[4] *Polariton condensation in photonic molecules*, M. Galbiati, et al., Phys. Rev. Lett. 108, 126403 (2012);
[5] *Propagation and Amplification Dynamics of 1D Polariton Condensates*, E. Wertz et al., Phys. Rev. Lett. 109, 216404 (2012).
[6] *Macroscopic quantum self-trapping and Josephson oscillations of exciton-polaritons*, M. Abbarchi et al., Nature Physics 9, 275(2013).
[7] *Polariton condensation in solitonic gap states in a one-dimensional periodic potential*, D. Tanese et al., Nature Communications 4, 1749 (2013).
[8] *Realization of a double barrier resonant tunneling diode for cavity polaritons,* H-.S. Nguyen et al., Phys. Rev. Lett. 110, 236601 (2013).

ORALES

Sesión 1: Grafeno y otros sistemas de baja dimensionalidad

Miércoles 22, 10:00 (invitada)

Optical nano-imaging of gate-tuneable graphene plasmons

Pablo Alonso-González[1,*], Jianing Chen[5,1], Michela Badioli[2], Sukosin Thongrattanasiri[3], Florian Huth[1,6], Johann Osmond[2] M r o p senovi [2], Alba Centeno[7], Amaia Pesquera[7], Philippe Godignon[8], Amaia Zurutuza[7], Nicolas Camara[9], Javier Garcia de Abajo[3], Rainer Hillenbrand[1,4], Frank Koppens[2]

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[2]*ICFO-Institut de Ciéncies Fotoniques, Mediterranean Technology Park, 08860 Castelldefels (Barcelona), Spain*
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[4]*IKERBASQUE, BasqueFoundationforScience, 48011, Bilbao, Spain*
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Graphene holds great promise for ultra-compact and electronically controlled plasmonics. Recently, resonant coupling of propagating THz waves to plasmons in micro-ribbons has been demonstrated, while IR near-field microscopy has been applied to observe the coupling of graphene plasmons to phonons. In our work [1] we use (similar to ref. [2]) scattering-type scanning near-field optical microscopy (s-SNOM) to visualize propagating and localized infrared plasmon modes in graphene nanostructures in real space (Fig. 1). By spectroscopic im ging we me sure the gr phene pl smon w velength λ_p s function of excit tion wavelength, which confirms the theoretically predicted plasmon dispersion. We observe that the pl smon w velength $\lambda_p=\lambda_0/40$ is remarkably reduced compared to the illumin tion w velength λ_0, which can directly be attributed to the two-dimensionality and unique conductance properties of graphene. Furthermore, we demonstrate tunability of the plasmon wavelength by gating graphene nanoribbons on a SiO_2 substrate. The possibility to tune plasmons of extreme subwavelength electronically opens up a new paradigm in optical and opto-electronic telecommunications and information processing.

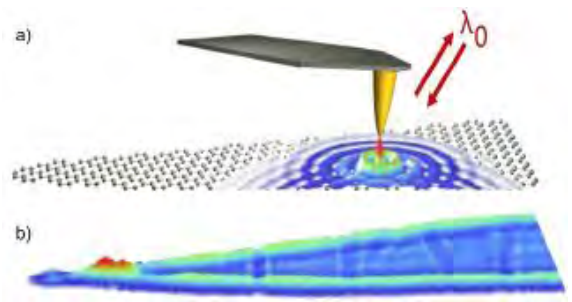

Fig 1. Imaging propagating and localized graphene plasmons by *s*-SNOM. a) Schematic of the experimental configuration used to launch and detect propagating surface waves in graphene. b) Near-field amplitude image acquired for a tapered graphene ribbon on top of 6H-SiC.

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[2] Z. Fei, et al., Nature **487**, 82 (2012)

Miércoles 22, 10:20 (invitada)

Nanomechanics and strain engineering in atomically thin MoS_2

Andres Castellanos-Gomez[1,*]

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Single-layer MoS_2 is an attractive two-dimensional material that combines the mechanical flexibility of graphene with a large direct bandgap. While graphene is very interesting as a transparent electrode, its lack of a bandgap limits its usefulness in semiconducting and optoelectronic devices. Atomically thin MoS_2, on the other hand, has a large intrinsic bandgap. This attractive feature has been employed to fabricate many devices not possible in graphene, such as field-effect transistors with high mobility and current on/off ratio, logic gates and efficient photo-transistors. Our recent work on MoS_2 has been focused on developing new methods to fabricate single layer MoS_2 [1] and to characterize the intrinsic mechanical [2], optical and electrical properties [3-4] of this atomically thin material.

Here, I will show an overview of our lastest results on MoS_2 paying special attention to our studies on nanomechanical resonators based on MoS_2 layers [5] and on the effect of localized strain on the optoelectronic properties of MoS_2 [6].

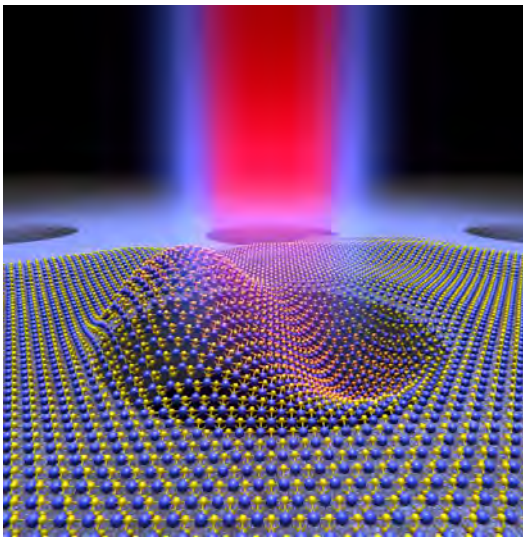

Fig 1. A focalized laser is used to detect the oscillation of a MoS_2 layer suspended over a hole, creating a microscopic drumhead.

[1] Castellanos-Gomez, A., et al., *Laser-Thinning of MoS2: On Demand Generation of a Single-Layer Semiconductor.* Nano Letters, 2012. **12**(6): p. 3187-3192.
[2] Castellanos-Gomez, A., et al., *Elastic Properties of Freely Suspended MoS2 Nanosheets.* Advanced Materials, 2012. **24**(6): p. 772-775.
[3] Castellanos-Gomez, A., et al., *Electric-Field Screening in Atomically Thin Layers of MoS2: the Role of Interlayer Coupling.* Advanced Materials, 2013. **25**(6): p. 899-903.
[4] Buscema, M., et al., *Large and Tunable Photothermoelectric Effect in Single-Layer MoS2.* Nano Letters, 2013.**13** (2), p. 358–363
[5] Castellanos-Gomez, A., et al., *Single-layer MoS2 mechanical resonators.* Advanced Materials, 2013 (DOI: 10.1002/adma.201303569).
[6] Castellanos-Gomez, A., et al., *Local strain engineering in atomically thin MoS2.* Nano Letters 2013 (DOI: 10.1021/nl402875m).

Miércoles 22, 10:40 (invitada)

Looking for quantum size effects in bismuth thin films and nanowires

L. Perez[1,*], M. Plaza[2], S. Sangiao[3], M. Abuín[1], A. Prados[1], M. C. Martínez-Velarte[4,5], N. Marcano[4,5], M. C. Sánchez[1], M. A. Gonzalez-Barrio[1], A. Mascaraque[1], L. Morellón[4,5] and J. M. de Teresa[5,6]

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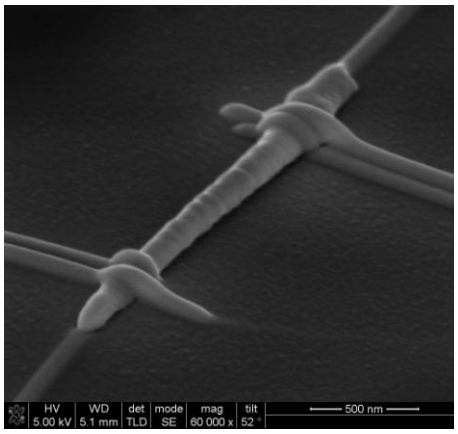
Bismuth (Bi) has received ample attention in the last decades due to its unique electronic properties, which arise from the highly anisotropic Fermi Surface. Its long electron Fermi wavelength makes Bi one of the most suitable scenarios for the study of Quantum Size Effects (QSE) in 1D and 2D systems. Recently, the appearance of highly-metallic surface states in Bi thin films, states that are strongly spin polarized, makes this material an interesting candidate for spin-related applications.

We will present our more recent results in the synthesis and characterization of Bi nanomaterials (nanowires and thin films). On one hand, we have electrodeposited single crystal nanowires and contacted an individual nanowire by means of Focus Ion Beam Induced Deposition (FIBID) as shown in the figure. A three band model is needed to fit the magnetoresistance measurements below 100 K, which can be explained by the presence of a robust metallic surface state. Magnetoresistance measurements also show evidence for weak antilocalization at temperatures below 10 K [1].



Bismuth nanowire contacted via FIBID for magnetotransport measurements.

On the other hand, we have studied the magnetotransport properties of polycrystalline ultrathin films of Bi grown on thermally oxidized Si(001) substrates with thickness ranging from 10 to 100 nm, finding remarkable differences in both in temperature and field dependence of the Hall resistivity with thickness above and below 20 nm. These results can also be explained due to the presence of surface states. We have estimated the surface carrier density, which correlates well with values from Angle-Resolved Photoemission Spectroscopy (ARPES) in ultrathin Bi films [2].

We will also present our results on the epitaxial growth of Bi layers on n-GaAs substrates [3]. Although these results should be improved to allow magnetotransport measurements without current leakages through the substrate, it seems to be an interesting route to keep exploring QSE and surface states in Bi nanostructures.

[1] N. Marcano et al., Appl. Phys. Lett, 2010, 96, 082110.
[2] N. Marcano et al. Phys. Rev. B, 2010, 82, 125326.
[3] M. Plaza et al. Mat. Chem. Phys. 134 (2012) 523-530.

Miércoles 22, 12:20

Experimental evidence for Topological Insulator behaviour in atomic layers of Bismuth (111) at room temperature

C. Sabater[1,3*], T. Urata[1], M. Neklyudova[2], D. Gosálbez-Martínez[3], J. Fernández-Rossier[4], J. G. Rodrigo[5], C. Untiedt[3], J. J. Palacios[5], H.W. Zandbergen[2], J.M. van Ruitenbeek[1]

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[3]Universidad de Alicante, Departamento de Física Aplicada, San Vicencte del Raspeig, Alicante 03690, Spain
[4]Internacional Iberian Nanotechnology Laboratory, Avenida Mestre José Veiga, Braga 4716-330, Portugal
[5]Universidad de Autónoma Madrid, Departamento de Física de la Materia Condensada and Instituto de Física de la Materia Condensada (IFIMAC) , Cantoblanco, Madrid 28049, Spain

A single bilayer of bismuth oriented in the crystallographic direction (111) was proposed by Murakami as a 2-dimensional material with Quantum Spin Hall states. One of the distinguishing properties for this 2 dimensional Topological Insulators material is that its electronic transport is at one quantum unit of conductance ($G_0=2e^2/h$). Through electrical conductance measurements of Bi nanocontacts created by repeated indentation using STM at room temperature we have observed values of conductance close to 1 G_0 for up to hundreds of nanometers in the retraction process between the electrodes. This suggests that a large structure, possibly a Bi (111) atomic layer, would be produced by mechanical exfoliation.

Through High Resolution Transmission Electron Microscopy combined with measurements of electronic transport in Bismuth atomic layers, we have found additional , although indirect, evidence of quantum Spin Hall behaviour. Our findings provide the first experimental evidence of the possibility of mechanical exfoliation of Bi bilayers, of the existence of the QSH phase in a two-dimensional Bi crystal, and, most importantly, of the observation of the QSH phase at room temperature.

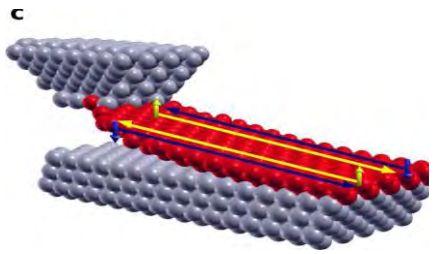

Fig 1. Pictorial representation of the proposed process of exfoliation of a Bi(111) bilayer after contact with the STM tip.

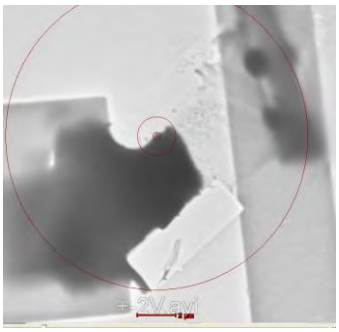

Fig 2. High Resolution Transmision Electron Microscope image on Bismuth thin flake which conductance is close to 1 G_0.

[1] S. Murakami Physical Review Letters **97**, (2006) 236805.
[2] C. Sabater *et al.* Physical Review Letters, **110,** (2013) 176802.

Miércoles 22, 12:40

Graphene derivatives from Ball-milling of graphite

V. León[1,*], M. Prato[2], E. Vazquez[1]

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[2]*Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste, Piazzale Europa, 1. 34127 Trieste (Italy).*

The emergence of graphene has recently opened up a new field in the science and technology of two-dimensional nanomaterials with continuously growing interest. Graphene exhibits unique properties arising from its strictly single atomic layers of sp^2-bonded carbon atoms densely packed in a honeycomb crystal lattice. These properties generate huge interest from different application fields,[1] however they are also highly dependent on the number of layers of graphene. Unless well separated from each other, graphene tends to form irreversible agglomerates or recovers to form graphite through Van der Waals interactions.[2] Therefore, stable dispersion of individual graphene sheets, in convenient media, is essential for the material to be fully exploited in the different application fields.

Recently, our research group has developed a scalable and easy methodology for the exfoliation of graphite sheets through interactions with melamine (2,4,6-triamine-1,3,5-triazine) by ball milling processes in solvent free conditions. The milling treatments can be modulated in order to achieve graphene flakes with different sizes. Once graphite is exfoliated, the graphene layers can be dispersed in water and organic solvents at room temperature, by means of soft sonication conditions. Moreover melamine can be removed by filtration and graphene samples are redispersed in fresh solvents forming stable dispersions during weeks.[3]

The methodology opens the way for an efficient processing of these materials. Once dispersions are obtained, it is possible to deposit graphene onto different surfaces; moreover, graphene dispersions can be used in the preparation of new polymer composites.

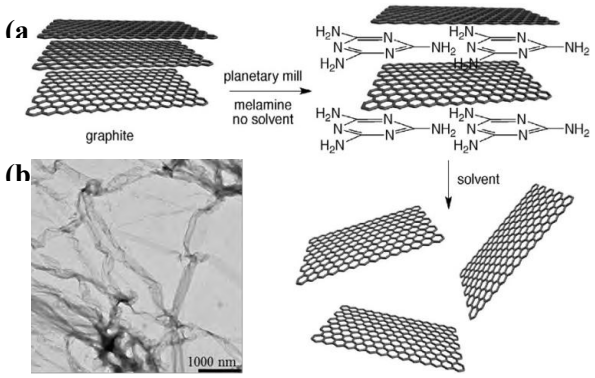

Figure 1. (a) Schematic illustration for the exfoliation of graphite through a ball-milling approach. (b) TEM image of exfoliated graphene.

[1] P. Avouris and C. Dimitrakopoulos, Materials Today, **15**, (2012) 86
[2] S. Park and R. S. Ruoff, Nature Nanotechnology, **4**, (2009) 217.
[3] V. León, M. Quintana, M. A. Herrero, J. L. G. Fierro, A. de la Hoz, M. Prato and E. Vázquez, Chemical Communications, **47**, (2011) 10936.

Miércoles 22, 13:00

Floquet-Bloch theory, irradiated graphene and topological phases

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[1]*Instituto de Ciencia de Materiales, CSIC, Cantoblanco, Madrid E-28049, Spain*
[2]*Département de Physique Théorique, Université de Genève, CH-1211 Genève, Switzerland*

We will describe the general properties which arise in periodically driven systems, with a special focus on the topological phases. We will show how suitable drivings, allow to tune the microscopic parameters of the undriven system, or even simulate topological structures which are unreachable for its time independent counterpart **[1]**. Next we show how this technique can be applied to a dimers chain (such as Polyacetylene), which is one of the main systems studied in physics due to its suitability to describe some non-trivial topological phases. Finally, we discuss how an AC electric field, coupled to electrons inthe a honeycomb lattice, influences their electronic structure, proving the possibility to merge the Dirac cones, as well as increase their number**[2]**, or simulate a Chern insulator (realization of the Haldane model) with tunable Chern number**[3]**.

[1] Á Gómez-León, G. Platero, Physical Review Letters **110** (20), 200403 (2013).
[2] P. Delplace, Á. Gómez-León, G. Platero, arXiv preprint arXiv: 1304.6272 (2013).
[3] Á. Gómez-León, P. Delplace, G. Platero, arXiv preprint arXiv: 1309.5402 (2013).

Miércoles 22, 13:20

Carbon nanostructures: application perspectives from the commercial point of view

José Luis Valverde Palomino

Departamento de Ingeniería Química, UCLM-Ciudad Real. Asesor de la empresa GRAPHENANO

The singular properties of graphene and other carbon nanostructures has opened up new horizons to the scientific community which will lead to new applications in fields like communications, medicine, electronics, etc., allowing new products to change the way we will interact with the technology and the nature. The aim of this presentation is to introduce the nanotechnology products that manufacture the company GRAPHENANO: graphene, carbon nanofiber, carbon nanospheres and aerogels. Some considerations on the procedure of scaling up manufacture, real demand, from the viewpoint of this company, and future developments, according to that demand, will be analysed.

ORALES

Sesión 2: Propiedades físicas de sólidos en la nanoescala, física de superficies e intercaras, microscopías de proximidad y microscopía electrónica

Miércoles 22, 15:20 (invitada)

Theoretical STM Characterization of Organics on Surfaces

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[1]*Dept. de Superficies y Recubrimientos (ICMM / CSIC), ES-28049 Madrid, Spain*

Understanding the interaction between organic molecules and surfaces is of paramount importance in diverse fields such as organic electronics, molecular electronics, catalysis, and surface photochemistry, among others. In particular, the growing field of organic electronics relies on the use of organic conjugated molecules as components of multilayer devices. For this purpose, an accurate theoretical Scanning Tunelling Microscopy approach arises as a powerful tool for a full structural and electronic characterization of organic molecules on surfaces, and establishes an excellent link between experiments and theory.

On the basis of the Unified IDIS model, an accurate Keldish-Green-based theoretical scanning tunneling microscopy approach [1] has been used to fully characterize the interaction between a large variety of organic molecules – such as Bz [2a], TTF [2b], TCNQ [2c], PTCDA [2d, 2e], Perylene, C_{60}, and some Heteroaromatics ($C_{60}H_{24}N_2$ and $C_{60}H_{30}$) [3,4] – with essentially different substrates, such as Au(111), Pt(111), TiO_2(110) and supported graphene. These molecules are prototypical electron donors and acceptors, and are in potentials of catalysis and molecular electronics as active catalysts precursors, promising candidates of organic conductors, and some of them interesting due to their hole-injection barrier found on a variety of polycrystalline substrates. On the other hand, recent investigations by our group have proved that thermal-induced (cyclo)dehydrogenation leads some Heteroaromatic PAH precursors to the formation of pristine or N-doped graphene [3,4]. Our theoretical STM approach has been used to characterize such systems, exhibiting an excellent agreement with the experimental evidence. As limit case of metal/organic interfaces, we have fully characterized the formation of Moiré superstructures in graphene layers on Pt surfaces.

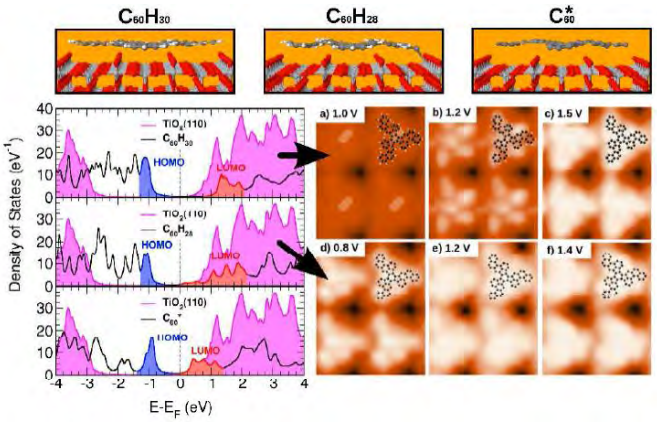

Fig 1. Density of states and theoretical STM images along the temperatura-assisted (cyclo)dehydrogenation process of the $C_{60}H_{30}$ PAH on TiO_2(110) [4].

[1] J. M. Blanco *et al.*, *Phys. Rev. B* **70**, (2004) 085405.
[2] a) J. I. Martínez *et al.*, *J. Chem. Phys.* **134**, (2011) 044701; b) *Org. Elec.* **13**, (2012) 399; c) *Phys. Stat. Sol. B* **248**, (2011) 2044; d) *Chem. Phys.* **390**, (2011) 14; e) *Phys. Rev. Lett.* **108**, (2012) 246102.
[3] A. L. Pinardi, J. I. Martínez, J. A. Martín-Gago *et al.*, *ACS Nano* **7(4)**, (2013) 3676.
[4] C. Sánchez-Sánchez, J. I. Martínez, J. A. Martín-Gago, *Nanoscale* **5**, (2013) 11058.

Miércoles 22, 15:40 (invitada)

Direct Imaging of Covalent Bond Structure in Single-Molecule Chemical Reactions

D. G. de Oteyza[1,2*], Y.-C. Chen[1,3], P. Gorman[4], S. Wickenburg[1,3], A. Riss[1], D. J. Mowbray[5,6], G. Etkin[4], Z. Pedramrazi[1], H.-Z. Tsai[1], A. Rubio[2,5,6], F. R. Fischer[4], M. F. Crommie[1,3]

[1] *Department of Physics, University of California at Berkeley, Berkeley, USA*
[2] *Centro de Física de Materiales CSIC/UPV-EHU, San Sebastián, Spain*
[3] *Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA*
[4] *Department of Chemistry, University of California at Berkeley, Berkeley, CA, USA*
[5] *Donostia International Physics Center (DIPC), San Sebastián, Spain*
[6] *Nano-Bio Spectroscopy Group and ETSF Scientific Develoment Center, Dpto. de Física de Materiales, Universidad del País Vasco UPV/EHU, San Sebastián, Spain*

Observing the intricate chemical transformation of an individual molecule as it undergoes a complex reaction is a long-standing challenge in molecular imaging. Advances in scanning probe microscopy now provide the tools to visualize not only the frontier orbitals of chemical reaction partners and products, but their internal covalent bond configurations as well. We have used non-contact atomic force microscopy to investigate reaction-induced changes in the detailed internal bond structure of individual oligo-(phenylene-1,2-ethynylenes) on a (100) oriented silver surface as they underwent a series of cyclization processes (Fig. 1). Our bond-resolved single-molecule imaging, together with DFT calculations, allows us to extract an exhaustive picture and unparalleled insight into the chemistry involved in complex enediyne cyclization cascades on Ag(100) surfaces.[1] The detailed mechanistic understanding can in turn guide the design of precursors for the rational synthesis of functional molecular architectures by means of surface-supported chemistry. [2] This approach represents an alternative route to get complex molecular building blocks onto surfaces.

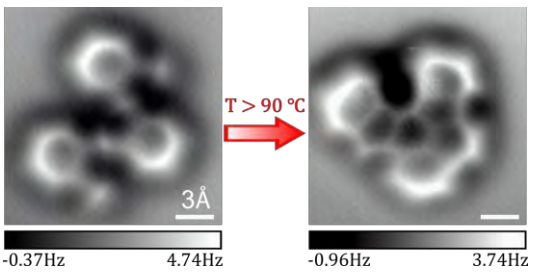

Fig 1. nc-AFM images of the precursor on Ag(100) before and after (product) chemical reaction.

[1] D. G. de Oteyza, P. Gorman, Y.-C.Chen, S. Wickenburg, A. Riss, D. J. Mowbray, Z. Pehdramrazi, H.-Z. Son, G. Etkin, A. Rubio, M. F. Crommie, F. Fischer, Science **340**, (2013) 1434.
[2] A. Riss, S. Wickenburg, P. Gorman, L. Z. Tan, H.-Z. Son, D. G. de Oteyza, Y.-C.Chen, A. J. Bradley, M. M. Ugeda, G. Etkin, S. G. Louie, F. Fischer, M. F. Crommie, Submitted.

Miércoles 22, 16:00

Exchange Bias Effect in $CoO@Fe_3O_4$ core-shell octahedron-shaped nanoparticles

Nerio Fontaíña Troitiño,[1] Beatriz Rivas Murias,[2] Benito Rodríguez González,[1] Francisco Rivadulla,[2] Verónica Salgueiriño[1]*

[1] *Departamento de Física Aplicada and CACTI, Universidade de Vigo, 36310, Vigo (Spain)*
[2] *Centro de Investigación en Química-Biológica y Materiales Moleculares (CIQUS), c/Jenaro de la Fuente s/n, Campus Vida, 15782-Santiago de Compostela, Spain*

Increased coercivity and tunable exchange bias field values were measured in hybrid $CoO@Fe_3O_4$ core-shell octahedron-shaped nanoparticles considering two different average edge length of the antiferromagnetic cores and two different thicknesses of the ferrimagnetic shell. The magnetic hardness attained after growing epitaxially the magnetite shell onto the CoO {111} surface facets just underlines the different parameters playing a role in the type of interface established and the consequent tunability of the exchange bias effect registered.

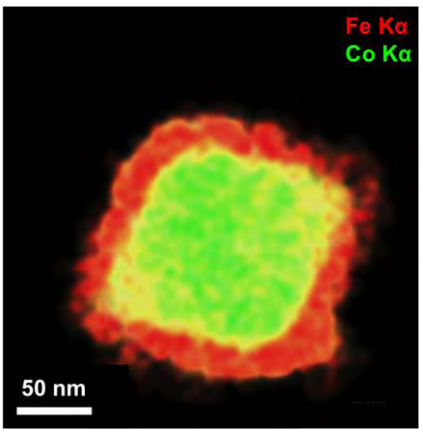

Fig 1. HAADF-STEM image and EDS elemental mappings showing the distribution of the Co, Fe and O within the particles.

[1] N. Fontaíña-Troitiño, B. Rivas-Murias, B. Rodríguez-González, F. Rivadulla, V. Salgueiriño (in preparation, 2013).

Miércoles 22, 16:20

Strain-induced ferromagnetism in $LaCoO_3$ and interface coupling in magnetic multilayers

Beatriz Rivas-Murias,* Irene Lucas[‡,1,2], Pilar J. Cavero[1,2], Andrey Chuvilin[†], Luis Hueso[†], Luis Morellon[1,2], Francisco Rivadulla

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[‡] Fundación ARAID, 50004 Zaragoza, Spain
[1] Instituto de Nanociencia de Aragón, Universidad de Zaragoza, 50018 Zaragoza, Spain
[2] Departamento de Física de la Materia Condensada, Universidad de Zaragoza, 50009 Zaragoza, Spain
†CIC nanoGUNE, Avenida de Tolosa 76, 20018 San Sebastian, and IKERBASQUE, Basque Foundation for Science, Bilbao.

Ferromagnetic insulators (FI) are scarce in nature, but have an important role in microwave applications, magnetooptics or in the fabrication of spin-filter tunnel barriers in spintronics. Electron tunneling across these barriers will depend on the relative orientation of the majority spins of the barrier and the injected electrons. An interesting example of a FI is the case of strained thin films of $LaCoO_3$ (LCO). In its bulk form, LCO adopts a rhombohedral structure, with the Co^{3+} atoms in a low spin (LS) diamagnetic configuration $t_{2g}^6e_g^0$. However, the intraatomic exchange splitting is of similar energy to the crystal field of Co^{3+} in an octahedral oxygen environment (≈20-80 meV), and a continuous transition between the LS and the high-spin (HS, $t_{2g}^4e_g^2$, S=2), configuration can be induced by epitaxial tensile stress.[1]

We have grown ultrathin films of LCO (≈2 nm) on top of $SrTiO_3$ (STO, ≈1.5 nm) and $La_{2/3}Sr_{1/3}MnO_3$ (LSMO, ≈22 nm). Magnetization and conductive AFM (C-AFM) transport experiments in the trilayer demonstrate that the ferromagnetic insulating behavior is kept in ultrathin LCO, with a T_C≈90 K, and M≈0.8 μ_B/Co. We show that the magnetization of LCO and LSMO is decoupled by the STO barrier, and so can be independently switched. C-AFM experiments performed using the nanostencil technique to deposit contacts on the surface in the range of 5μm to 10 μm diameter show I-V curves characteristic of tunnel conduction between the ferromagnetic electrodes across the STO barrier. Moreover, the magnetization of both layers can be conveniently coupled/decoupled by changing the order of deposition of the films (either LCO/LSMO or LSMO/LCO). These results show that new approaches for the design of insulating ferromagnets are possible.

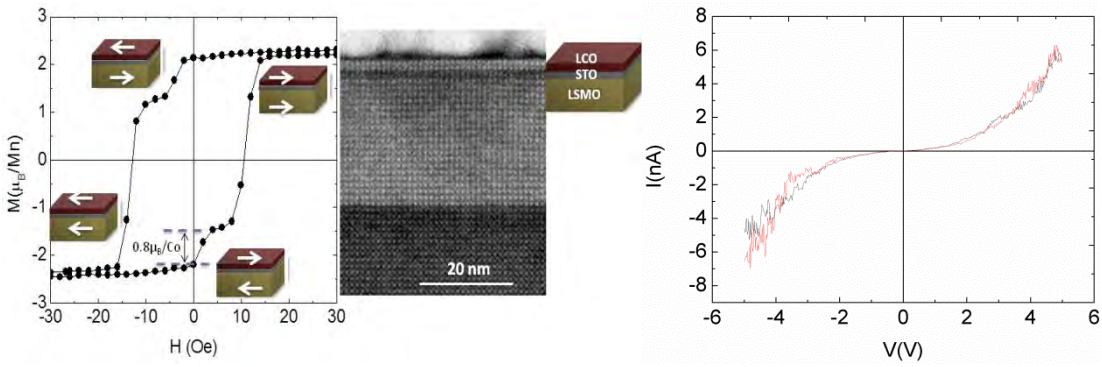

Figure. Left: Hysteresis loop at 10K of the LSMO/STO/LCO trilayer, showing the independent switching of the magnetization of the LCO and LSMO layers. A high resolution TEM picture of the film is shown in the middle panel. Rigth: I/V curves of the trilayer.

[1] D. Fuchs, et al. Phys. Rev. B **75**, (2007) 144402.

Miércoles 22, 16:40

Contrast Mechanisms on a Metal-Oxide Surface: Towards Chemically Selective Imaging by Controlling Tip-Apex Chemistry

M. Todorovi [1,*], H. Mönig[2], M. Z. Baykara[3], T. C. Schwendemann[4], L. Rodrigo[1], E. I. Altman[5], U. D. Schwarz[5] and R. Pérez[1]

[1]*Universidad Autónoma de Madrid, Dpto. Física Teórica de la Materia Condensada, 28049 Madrid, Spain*
[2]*Westfälische Wilhelms-Universität Munster-CeNTech ,48149 Munster, Germany*
[3]*Bilkent University, Department of Mechanical Engineering, 06800 Ankara, Turkey*
[4]*Southern Connecticut State University, Department of Physics, CT 06515 New Haven, USA*
[5]*Yale University, School of Engineering and Applied Science, CT 06520 New Haven, USA*

In the present study on a model high-symmetry Cu(100)-O surface, we combine STM experiments with density-functional theory (DFT) and Non-Equilibrium Green's Function (NEGF) calculations [1] to investigate the role of tip apex chemistry in contrast formation mechanisms and understand how it may be exploited to achieve functional imaging. At the outset, we systematically applied calculations to explore the STM imaging characteristics of Cu-O tips with different chemical terminations as a function of STM tip height and bias voltage. We were able to identify the imaging modes of tips terminating in a metal, non-metal and an intermediate adatom-contamination geometry and interpret them in terms of the contrasting tunnelling properties of Cu and O chemical species for a range of typical experimental parameters. Simulated imaging of a high-symmetry surface with asymmetric tip structures produced insight into asymmetric image features, STM image offsets and the imaging of surface domains on Cu(100)-O.

Based on these results, we conducted an extensive comparison of the computed STM image database with the bank of experimental images. We found remarkable agreement, which validated the chosen tip models. Our simulations show that dynamic contamination of metallic tips on the Cu(100)-O surface is highly likely, leading to STM image offsets and varied asymmetry effects observed in experiments [2]. O-terminated tips were particularly stable and frequently identified in experimental images: our simulations of their conducting properties show their imaging mode could be experimentally manipulated to selectively image metallic or non-metal surface species. By providing a comprehensive understanding into STM contrast formation mechanisms, we suggest how controlled changes in tip apex chemistry could be employed to enhance the functionality of SPM probes, thus allowing in-depth, species-specific analysis of complex compounds.

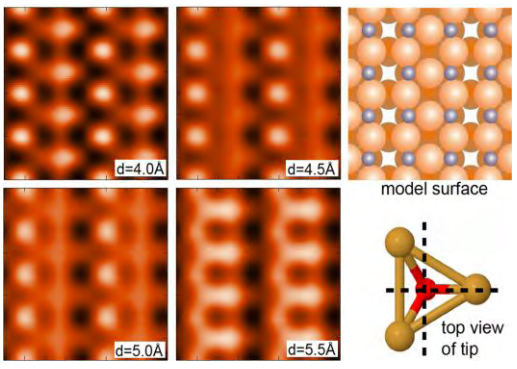

Figure 1: STM contrast variation with CuO tip approach from 5.5Å to 4.0Å (V=+0.4V), shown alongside the Cu(100)-O surface schematic and the top view of the tip.

[1] J. M. Blanco, F. Flores and R. Pérez, Prog.Surf. Sci. 81, (2006), 403.
[2] H. Mönig, M. Todorovi *et al*., ACS Nano (2013), doi:10.1021/nn4045358.

Miércoles 22, 17:00

Tunneling magnetoresistance in Fe/MgO/$La_{0.7}Sr_{0.3}MnO_3$ magnetic tunnel junctions

R. Galceran[1,*], Ll. Balcells[1], B. Bozzo[1], J. Cisneros[1], M. de la Mata[1], J. Arbiol[1], B. Martínez[1], J. Tornos[2], F. A. Cuellar[2], Z. Sefrioui[2], J. Santamaría[2], A. Cebollada[3], F. Golmar[4], F. Casanova[4], C. Martinez-Boubeta[5]

[1]*Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus de Bellaterra, 08193 Cerdanyola del Vallès, Spain*
[2]*GFMC. Depto. Fisica Aplicada III. Facultad de Fisica. Universidad Complutense, 28040 Madrid, Spain*
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[4]*CIC nanoGUNE Consolider, Tolosa Hiribidea 76, 20018 Donostia-San Sebastian, Spain*
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The performance of devices based on magnetic tunnel junctions heavily relies on interfacial properties. In this presentation we will comment on the magnetotransport properties of Fe/MgO/$La_{0.7}Sr_{0.3}MnO_3$ (LSMO) magnetic tunnel junctions, which are expected to present a considerably high and positive tunneling magnetoresistance (TMR) due to the half-metallic character of LSMO and the spin filtering properties of the MgO barrier [1]. We note, however, that the spin filtering effect through the Fe/MgO system depends critically on the quality of the interface.

Our experimental results allow identifying positive and negative contributions to the tunneling magnetoresistance (see Fig. 1), which suggests the existence of a ferromagnetic oxide layer at the Fe/MgO interface, possibly Fe_3O_4 [2]. We put forward the hypothesis that the TMR displays different signs depending on the role of this iron oxide layer (for example, acting as an intrinsic barrier or electrode). In our view, the TMR dependence on parameters such as the temperature range of the measurement (revealing a metal-insulator transition in the iron oxide) and the voltage applied to the junction lends support to our hypothesis. The possibility of anisotropic magnetoresistance of the iron oxide being responsible for the negative magnetoresistance must also be taken into consideration. However, to discuss this point, evaluation of Fe/Mg/MgO/LSMO junctions is required in future work.

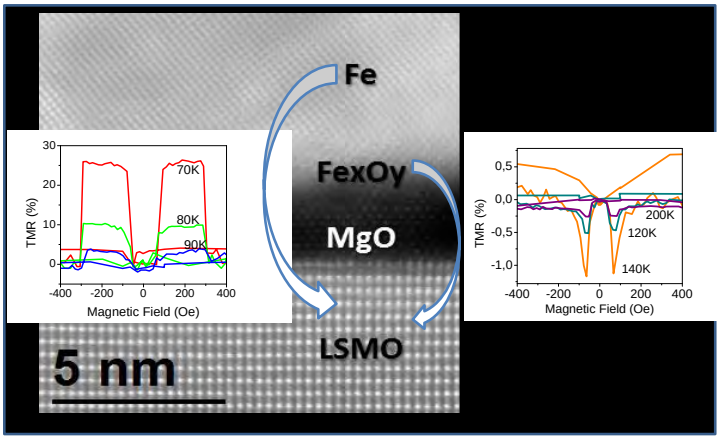

Fig 1. Transmission electron microscopy image of the cross-section of the junction, together with the interpretation of the temperature dependence of the magnetoresistance change of sign.

[1] W. H. Butler, X. G. Zhang, T. C. Schulthess, and J. M. MacLaren, Phys. Rev. B **63**, (2001) 054416
[2] C. Martinez-Boubeta, Ll. Balcells, S. Valencia, D. Schmitz, C. Monty and B. Martínez, Applied Physics Letters **94**, (2009) 262507.

Miércoles 22, 17:20

High performance MoS_2 Field-Effect Transitors in a simple design

S. Vélez[1,*], O. Txoperena[1], L. Pietrobon[1], F. Casanova[1,2], L. E. Hueso[1,2]

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The discovery of graphene [1], with its rich and fascinating physical properties [2], has opened up a new world where 2D-layered materials is the platform for developing powerful devices. Molybdenum disulfide (MoS_2), a 2D material belonging to the family of transition metal dichalcogenides, has an intrinsic band-gap and strong spin-orbit coupling which would complement those applications pristine graphene cannot cover [3]. In particular, MoS_2 has been shown to work well as a field-effect transistor (FET) [4], to exhibit superconductivity [5] and valley polarization [6], demonstrating its potential in spintronics, valleytronics, or for designing other novel devices.

Here we will show high performance of FETs based on monolayer and a few layer MoS_2 working with a simple design (Si/SiO2 back gate and two terminal configuration). The FETs show room temperature ON/OFF ratios exceeding 10^7 and with mobilities higher than 10 $cm^2V^{-1}s^{-1}$. These values exceed previously reported ones in similar designs and support the viability of building up simpler but still powerful devices which would allow large scale fabrication suitable for nanoelectronics. Further investigations exploiting both spintronics and valleytronics of layered MoS_2 are the final goal of this work.

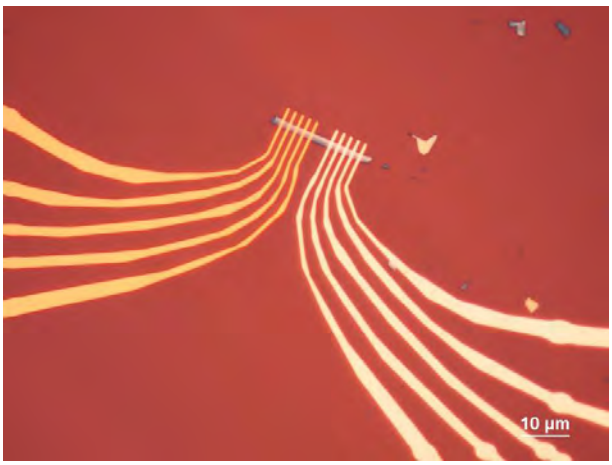

Figure: Optical image of a device fabricated based on a few layers flake of MoS_2

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[2] A. K. Geim & K. S. Novoselov, Nature Materials 6, 183 (2007); K. S. Novoselov et. al, Nature 490, 192 (2012).
[3] Q. H . Wang et al., Nature Nanotechnology **7**, 699 (2012).
[4] B. Radisavljevic et al., Nature Nanotechnology **6**, 147 (2011).
[5] K. Taniguchi et al., Applied Physics Letters 101, 042603 (2012); J. T. Ye, et al., Science 338, 1193 (2012).
[6] K. F. Mak et al., Nature Nanotechnology 7, 494 (2012); H. Zang et al., Nature Nanotechnology 7, 490 (2012); T. Cao et al., Nature Communications 3, 887 (2012).

** This work was financially supported by the European Research Council (Grant 257654-SPINTROS).

ORALES

Sesión 3: Materiales funcionales con aplicaciones en espintrónica, caloritrónica y energía.

Jueves 23, 10:00 (invitada)

Integrating functional oxide nanomaterials in silicon technology by chemical solution deposition

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In the past years, great efforts have been devoted to combine the functionality of oxides with the performances of semiconductor platforms for the development of novel and more efficient device applications. However, further incorporation of functional oxide nanostructures as active materials in electronics critically depends on the ability to integrate crystalline metal oxides into silicon structures. In this regard, the presented work takes advantage of all the benefits of soft chemistry to overcome the main challenges for the monolithic integration of novel nanostructured functional oxide materials on silicon including (i) epitaxial piezoelectric α-quartz thin films with tunable textures on silicon wafers [1] and (ii) 1D single crystalline phases of manganese oxide based nanostructures with enhanced ferromagnetic properties on silicon wafers that share common growth mechanisms [2].

Importantly, these mechanisms are governed by a thermally activated devitrification of the native amorphous silica surface layer assisted by a heterogeneous catalysis under atmospheric conditions driven by alkaline earth cations present in the precursor solution. Quartz films are made of perfectly oriented individual crystallites epitaxially grown on (100) face of Si substrate with a controlled porosity after using templating agents. Moreover, a quantitative study of the converse piezoelectric effect of quartz thin films through piezoresponse force microscopy shows that the piezoelectric coefficient d_{33} is between 1.5 and 3.5 pm/V which is in agreement with the 2.3 pm/V of the quartz single crystal d_{11}. Manganese based molecular sieve nanowires growth mechanism, involves the use of track-etched nanoporous polymer templates combined with the controlled growth of quartz thin films at the silicon surface, which allowed OMS nanowires to stabilize and crystallize. All together, the methodology presented here exhibits a great potential and offers a pathway to design novel oxide compounds on silicon substrates by chemical routes with unique optical, electric, or magnetic properties.

[1] A.Carretero-Genevrier et al. Science 340, (2013) 827
[2] A.Carretero-Genevrier et al. Chem.Soc.Rev. (2013) DOI: 10.1039/C3CS60288E.

Jueves 23, 10:20 (invitada)

Tailoring nanoparticles. Controlled size, composition and structure in a one-step process

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[2] *Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, Laboratorio de Microscopías Avanzadas (LMA), c/Mariano Esquillor, Edificio I+D, 50018 Zaragoza, Spain.*

There is an increasing demand of tailoring nanoparticles (NPs) for many different applications. In this talk we present a bottom-up fabrication route based on the sputtering gas aggregation source that allows the generation of nanoparticles with controllable and tunable chemical composition and structure while keeping the control of their size. This technique, called Multiple Ion Cluster Source (MICS) [1], is an evolution of standard Ion Cluster Sources (ICS) [2] that consist in the replacement of the single magnetron of the ICS by 3 small magnetrons completely independent (Figure 1).

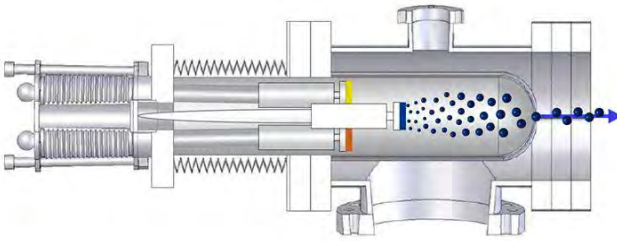

Fig 1. Scheme of the Multiple Ion Cluster Source.

Since the applied power and argon flux of each magnetron can be adjusted separately, the density of ions generated by each magnetron can be tuned continuously which leads to a fine control of the generated NPs. Therefore, it is possible to grow single nanoparticles or alloyed NPs with adjustable chemical composition and size [3]. Apart from this, as the relative positioning of the magnetrons inside the aggregation zone is also independent, it is possible to generate core-shell nanoparticles using two or the three magnetrons. All these possible combinations are generated in one single step process and under ultra-high vacuum (UHV) conditions, which leads to the formation of NPs with high purity. Figure 2 presents some examples of NPs fabricated with the MICS.

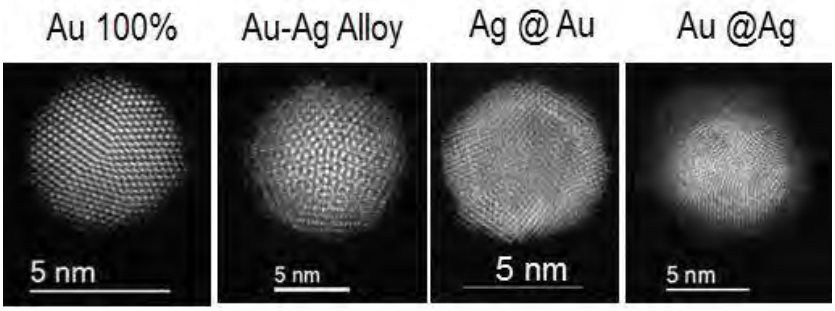

Fig 2. Examples of nanoparticles fabricated with the Multiple Ion Cluster Source.

[1] E. L. Román García, L. Martínez Orellana, M. Díaz Lagos, Y. Huttel (Oxford Applied Research Ltd.), *Spanish Patent P201030059*, **2010**.

[2] H. Haberland, M. Karrais, M. Mall, Z. Phys. D: At., Mol. Clusters, **20**, (1991) 413.

[3] L. Martínez, M. Díaz, E. Román, M. Ruano, D. Llamosa P., Y. Huttel, Langmuir, ***28***, (2012) 11241.

Jueves 23, 10:40 (invitada)

Solution processing of energy conversion materials and devices: photovoltaics and thermoelectricity

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Breakthroughs in materials hold the key to new generations of products. This breakthrough will be reached through the control of material properties and understanding of mechanisms and phenomena at the atomic scale. At the same time, industrial innovation will be supported on cost-effective technologies able to transform this control and understanding into optimized and new products.

In this scenario, solution-based methods allow production of nanomaterials with unmatched degree of control over size, shape, phase and composition of the crystalline domains. At the same time, the availability of materials in solution or in nano-ink forms enables large volume economic fabrication of devices over a variety of substrates by cost-effective printing and coating technologies.

We use solution-based synthesis routes and solution-processing thin film technologies to produce, at low cost, functional nanomaterials and films with nanometer-scale control over their composition, crystal phase, geometry and size. We use this nanomaterials and films to fabricate thermoelectric and photovoltaic devices.

In this seminar, I will talk about the challenges and advantages of solution processing techniques to produce efficient thin film photovoltaic devices and bulk nanostructured materials and the possibilities to overcome them.

Jueves 23, 12:20 (invitada)

Tuning the magnetic domain patterns of sputtered TbFeGa alloys

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The control of the magnetic domain patterns together with their time and temperature stability are key issues for the development of new devices. Materials systems with perpendicular magnetic anisotropy (PMA) are of great interest because of their applications on patterned media for magnetic storage or in spintronic devices [1]. Nowadays, different approaches are analyzed to reach this high magnetic anisotropy, leading to various structures such as FePt and CoPt layers, multilayers comprising magnetic transition metals (Co, Fe, CoFe) and noble metals (Pt, Pd, Au) or FeCoB layers with PMA.

Some years ago, Tb-Fe alloys were greatly investigated because of their large out-of-plane anisotropy constant [2]. In spite of this high PMA, for industrial applications it is desirable to have materials with a reduced heavy rare earth content. Some works on bulk TbFeGa alloys have focused on their magnetostrictive properties but it is only recently that the magnetic anisotropy of TbFeGa thin films has been studied [3-5].

In this work, we present our investigations on the magnetic properties of TbFeGa thin films. The alloys were obtained by the cosputtering technique using two targets with a composition of $TbFe_2$ and Fe_3Ga. Different compositions can be achieved by modifying the power in each sputtering target. Moreover, we have also observed that the magnetic anisotropy and domain patterns also depend on the type of power source used (DC or pulsed). In particular, the evaporation of $TbFe_2$ by means of the DC source enhances the out of plane component of the magnetization (Fig. 1) being obtained an anisotropy constant of at least 1×10^6 erg/cm^3. The results indicate that this is due to the Tb enrichment of the $TbFe_2$-based phases present in the alloys. Therefore, the magnetic domain pattern can be tailored by means of the composition and the type of power source used in each sputtering target.

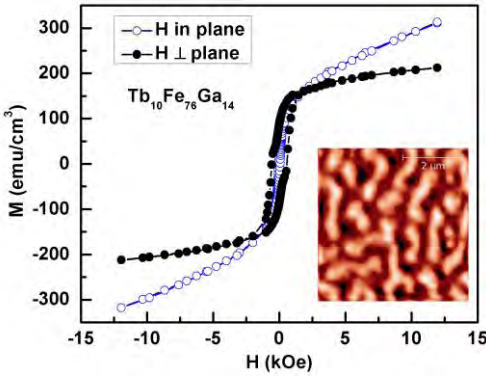

Fig 1. Room temperature hysteresis loops of the $Tb_{10}Fe_{76}Ga_{14}$ measured with the applied m gnetic field perpendicul r (●) nd in the s mple pl ne (○). Inset: MFM signal recorded at remanence.

[1] S. Mangin, D. Ravelosona, J. A. Katine, M. J. Carey, B. D. Terris, E. E. Fullerton, Nature Materials **5**, (2006) 210.
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[3] L. Jiang, J. Yang, H. Hao, *et al.,* Appl. Phys. Lett. **102** (2013) 222409.
[4] R. Ranchal, V. Gutiérrez-Díez, Thin Solid films **534**, (2013) 557.
[5] R. Ranchal, S. Fin, D. Bisero and C. Aroca, J. Alloys Compnd. **582**, (2014) 839.

Jueves 23, 12:40

Grain boundary effect on ionic transport in yttria stabilized zirconia

O. J. Durá[1,2], M. A. Frechero[1], M. Rocci[1], G. Sánchez-Santolino[1,3], Amit Kumar[5], J. Salafranca[1,3], Rainer Schmidt[1], M. R. Díaz-Guillén[1], A. Rivera-Calzada[1], M. A. López de la Torre[2],J Chaboy[4], R. Mishra[6,3], Stephen Jesse[5], M. Varela[3,1], S. T. Pantelides[3,6], Sergei V. Kalinin[5], S. J. Pennycook[3], J. Santamaria[1] and C. Leon[1]

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Yttria Stabilized Zirconia (YSZ) is widely used today as electrolyte in solid oxide fuel cells due to its high oxide ion conductivity at enough high temperature. The performance of this material in such devices is usually limited by its polycrystalline form, since ion blocking occurs at grain boundaries [1, 2]. Although this fact is well established, there is not general consensus yet on the understanding of grain boundary effects on ion transport through YSZ. In particular, the existence of space-charge effects at YSZ grain boundaries and its consequences on the ionic transport has been controversial during the last years. The differences between theoretical predictions and experimental findings have not helped to resolve the debate [3-5]. Here we present an exhaustive characterization of YSZ samples with very different microstructure where we have focused on the electrical behavior of the grain boundaries. We have characterized microcrystalline and nanocrystalline ceramic samples as well as polycrystalline thin films. We discuss experimental conductivity values in terms of a Schottky-like barrier at the grain boundaries, and obtain the electrostatic potential barrier ($\Delta\varphi$) as well as the space charge layer thickness (λ^*), and find important deviations from the theoretical predicted values. Finally we present a study of ionic transport through a single boundary in a YSZ bicrystal, where we confirm the electrostatic nature of the barrier for ion transport at grain boundaries. In addition, we find that $\Delta\varphi$ and λ^* values as determined from experimental data are in very good agreement with the theoretical predicted ones, although inconsistent with a Schottky model approximation. Our finding constitutes a key advance towards the understanding of ionic transport at interfaces, which will help in optimizing the performance of polycrystalline materials in solid state electrochemical devices.

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[5] O. J. Dura et al., Phys. Rev. B **87**, 174109 (2013).

Jueves 23, 13:00

Different routes for enhanced control of ferroelectric polarization by magnetic field

I. Fina[*,1,2], V. Skumryev[3,4] D.O'Flynn[5], G. Balakrishnan[5], N. Dix[2], J. M. Rebled[1,6], P. Gemeiner[7], X. Martí[8], F. Peiró[6], B. Dkhil[7], F. Sánchez[2], L. Fàbrega[2], J. Fontcuberta[2]

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[2]*Inst. de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra 08193, Catalonia, Spain*
[3]*Institució Catalana de Recerca i Estudis Avançats (ICREA), Catalonia, Spain*
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Multiferroic materials are those materials in which more than one ferroic order coexist. The most technologically appealing multiferroic materials are those showing ferromagnetism and ferroelectricity. The control of one of the ferroic orders by the complementary, called magnetoelectric coupling, can yield to new interesting functional applications. In spintronics this coupling would result in the possibility of building magnetic memories controlled by electric field, or, in electronics, transistors where charge is contact-less controlled by a magnetic field. I will focus on the direct magnetoelectric effect, control of polarization vector by magnetic field, in single-phase and composite materials.

In single-phase multiferroic materials the huge difference between the energy scales that involve magnetic and polar interactions hampers the possibility of having real control of ferroelectric polarization by magnetic field. We looked for this real control in cycloidal magnets, which show coupling between magnetic and ferroic order at low temperature, and we will see that the key is to take advantage of the competing magnetic interactions that these materials usually show and the fact that those result in a strong coexistence of polar and non-polar regions. This phase coexistence (sketch in figure 1(a)) allows large susceptibilities leading to a full control of the polarization vector by means of magnetic field [1].

In composite materials, the most feasible system is that where ferroelectric and magnetic layers are elastically coupled through interfaces in multilayer stacks. Here, the limiting factor is the substrate clamping effect. We studied bilayers of ferromagnetic and ferroelectric materials, and I will show that we can overcome the undesired clamping effect, enhancing the presence of some small quantity of defects. These defects store the needed elastic energy, reducing the clamping, and enhancing the magnetoelectric coupling (sketch in figure 1(b)), which result in huge effects near room temperature [2].

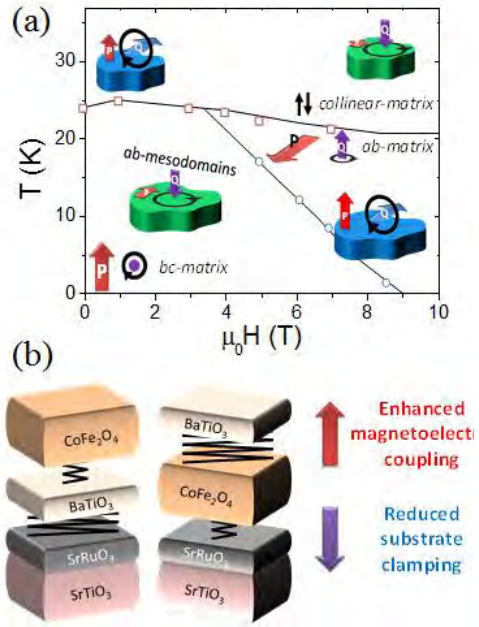

Figure 1. Sketch of the phase coexistance of different magnetic configuration in archetypical $Sm_{0.5}Y_{0.5}MnO_3$ cycloidal magnet. (b) Sketch of the resulting enhancement of the magnetoelectric coupling in a archetypical $BaTiO_3$ and $CoFe_2O_4$ composite multiferroic system, after reducing the substrate clamping effect (small spring between the layers).

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Jueves 23, 13:20

Ferroelectric control of spin transport in oxide magnetic tunnel junctions

J. Tornos[1,*], Y. H. Liu[3], G. Sanchez-Santolino[1], C. Munuera[2], S. G. E. te Velthuis[3], F. Mompean[2], M. Garcia-Hernandez[2], M. Varela[4,1], S. J. Pennycook[4], Z. Sefrioui[1], C. Leon[1], J. Santamaria[1]

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[2]*Instituto de Ciencia de Materiales de Madrid, ICMM- CSIC, 28049 Cantoblanco, Spain*
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Magnetic tunnel junctions with a ferroelectric barrier enable the control of spin dependent resistance by reversing ferroelectric polarization. These devices thus display four different resistance states by switching the relative magnetizations alignment of the ferromagnetic electrodes for both directions of the ferroelectric polarization (see Figure 1). We report here on La0.7Sr0.3MnO3(LSMO)/BaTiO3(BTO)/LSMO magnetic tunnel junctions with an ultra-thin BTO ferroelectric barrier. We have found very large tunnel electro-resistance (TER) close to 1000% at low temperatures. This is interpreted in terms of a variation of the effective barrier thickness due to a large modulation of electron density at the BTO/LSMO interface. Oxygen vacancies at the highly strained BTO/LSMO bottom interface encompass a doping effect by the associated electron density. The reversal of the ferroelectric polarization of the BTO causes accumulation or depletion of the electron density at the bottom interface to screen the polarization charges giving rise to a significant modulation of the width of the tunnelling barrier. Furthermore, for the down-polarization, for which lower resistance values are found, tunnel magnetoresistance (TMR) is also strongly depressed, as a result of a depolarization of the tunneling current. This TMR modulation might be related to the presence of an induced Ti magnetic moment in BTO at the interface, antiferromagnetically coupled to that of Mn in LSMO, as detected by x-ray magnetic circular dichroism (XMCD) measurements. Our results reveal the possibility to tune spin dependent transport by an electric field through the reversal of the ferroelectric polarization of the barrier.

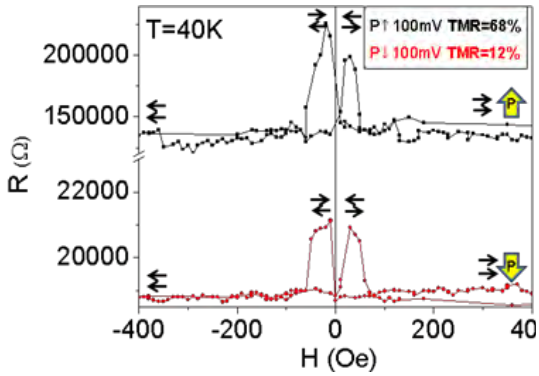

Fig 1. Junction resistance at 100 mV as a function of sweeping magnetic field for both ferroelectric polarization direction, up (black) and down (red).

ORALES

Sesión 4: Magnetismo, superconductividad, información cuántica, magnetismo y electrónica molecular, materiales complejos.

Jueves 23, 15:20 (invitada)

Intersite charge transfer and spin state transitions in Pr-based cobalt oxides by x-ray absorption/emission spectroscopies

J. Herrero-Martín[1,*], J. Padilla-Pantoja[2], and J. L. García-Muñoz[2]

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The electronic filling of the Co 3*d* valence band is key to the electronic and magnetic properties of cobaltites. The characteristic Co spin state (SS) degree of freedom is correlated to the electron mobility and it thus may play an important role in metal-insulator transitions (MITs).

MITs are found in a wide range of compositions of the $(Pr_{1-y}Y_y)_{1-x}Ca_xCoO3$ series, coupled to magnetic and structural changes. The low temperature insulating phase is characterized by the appearance of tetravalent Pr ions, accompanied by a striking crystal cell volume contraction [1,2]. X-ray absorption spectroscopy (XAS) data show that the electrons lost by Pr ions move to Co sites. The expected increase of the average Co-O distance is however not observed [3]. X-ray emission spectroscopy (XES) allows us to understand why: the occurrence of a concomitant Co SS change. The combination of these two spectroscopic techniques permits us to quantify these thermally induced electronic changes [4]. The photoexcited phase transition in $Pr_{0.5}Ca_{0.5}CoO_3$ (PCCO) when illuminated by laser radiation, where metallic domains can be stimulated [5], could then be related to induced SS changes.

The Ca by Sr alkali-earth substitution leads to the suppression of the MIT. We have also investigated metallic $Pr_{0.50}Sr_{0.50}CoO_3$ spectroscopically, which presents an anomalous transition at T_S~120 K, thought as owing to a large magnetostructural effect [6]. Despite not having observed any trace of Pr^{4+} in the wide thermal range studied, we point to an active participation of Pr ions across T_S. Similarly as in PCCO, noticeable associated bond contractions are observed, but XAS confirms the absence of any SS variation and shows the stability of the average formal valence of Co ions. The large density of empty t_{2g} symmetry states in the studied thermal range suggests to dismiss the occurrence of Co^{3+} in a pure low SS. The orbital filling configuration appears to be fundamental for the occurrence of the intersite charge transfer [7].

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[3] J. L. García-Muñoz *et al*, Phys. Rev. B **84** (2011) 045104; J. Herrero-Martín et al, Phys. Rev. B **84** (2011) 115131
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[5] Y. Okimoto et al, Phys. Rev. Lett. **103** (2009) 027402
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[7] J. Padilla-Pantoja *et al*, submitted

Jueves 23, 15:40 (invitada)

Magnetic properties of ionic liquids exhibiting three-dimensional magnetic order in their condensed phases

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The magnetic ionic liquids (MILs) are a new class of magnetic materials, which can favourably combine the properties of ionic liquids with the magnetism that is originated from the metal incorporated in the complex anion. These MILs are single component materials with unpaired electrons in the valence shell of the metal cation. In its condensed phase, the questions about cooperative magnetic effects, complex anion interaction, and magnetostructural correlation are quite important and it is actually in focus of materials science.

In this talk we present, the experimental and computational studies in MILs based on imidazolium cations. Most of the MILs are paramagnetic, being the Emim[$FeCl_4$] [1] and [Dimim][$FeCl_4$] [2] the first examples in which a long-range magnetic order was found at low temperatures. The physical properties clearly show antiferromagnetic ordering when they are solidified (in polycrystalline state), with a Neel temperatures below 10 K. Neutron powder diffraction experiments confirm the three-dimensional magnetic ordering in both compounds. In addition, it is observed that the pressure modifies the magnetic interactions in Emim[$FeCl_4$], increasing the order temperature and inducing a ferrimagnetic behaviour [3]. The magnetostructual correlations of [Dimim][$FeCl_4$] show that the formation of chlorine bridges allows the antiferromagnetic coupling, including two diamagnetic intermediaries. The results have been confirmed with computational studies displaying a large spin-density delocalization toward the chlorine atoms, which explains the efficiency of the superexchange pathways in transmitting the magnetic interaction [3].

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[2] A. García-Saiz, P. Migowski, O. Vallcorba, J. Junquera, J.A. Blanco, J. González, M. T. Fernández-Díaz, J. Rius, J. Dupont, J. Rodríguez Fernández and I. de Pedro, Chemistry A European Journal (to be published).
[3] A. García-Saiz, I. de Pedro, J. A. Blanco, J. González and J. R. Fernández, The Journal of Physical Chemistry B **117**, (2013) 3198.

Jueves 23, 16:00 (invitada)

Damping of quantum oscillations in the superconducting state of MgB_2

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The origin of quantum oscillations (QO) in the mixed state of type-II superconductors is an open issue of fundamental interest. A number of superconductors display QO below the upper critical magnetic field, H_{c2}. Most recently QO have been observed in the mixed state of underdoped cuprate superconductors. The frequency of the mixed state QO oscillations is always identical to those in the normal state but, in general, the amplitude shows an additional attenuation which theory suggests depends on the orbit averaged, field dependent superconducting gap. In principle then, the additional attenuation can be used to determine the field and momentum dependence of the superconducting gap. A case of particular interest is found in multiband superconductors where different gaps open over different sheets of the Fermi surface.

Here, I will discuss a de Haas-van Alphen study of the multiband superconductor MgB_2. In contrast to previous work [1], the samples in the present study are extremely clean (mean free paths in excess of 1000 Angstroms) and have negligible pinning. We have obtained first independent information about the high magnetic field dependence of the two superconducting gaps that open in the π and σ Fermi surfaces of this superconductor. In the π band, oscillations are visible well below H_{c2} and show very little additional damping, implying that the π Fermi surface superconducting gap has unconventional field dependence. In the σ band, oscillations are only visible at the so-called Yamaji angle where the two extremal orbits of the σ Fermi surface cross producing an enhancement in the amplitude of QO. The relation of our data to previous [1] results on more disordered samples will be discussed.

[1] J.D. Fletcher, et al., Phys. Rev. B **70**, (2004) 144501.

Jueves 23, 16:20 (invitada)

Quantum merging: a physical mechanism for non-Abelian quantum matter

Belén Paredes

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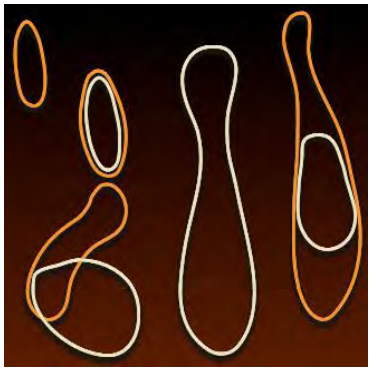
Topological states of matter represent an exotic organizational form of quantum matter that contradicts the traditional paradigms of condensed matter physics. Our understanding of how topological order emerges from the microscopic degrees of freedom of a quantum many-body system is far from complete. Especially intriguing is the possible formation of non-Abelian topological phases, whose excitations display non-Abelian braiding properties with potential application for quantum computing.

In this talk I will propose a physical mechanism for the emergence of non-Abelian topological phases: the quantum merging of identical copies of the same many-body state. I will argue that such a global organization, in which particles are organized into identical indistinguishable groups, can give rise to topological quasiparticles obeying non-Abelian statistics. To illustrate the construction, I will present a physical realization of this type of order in a spin-1 lattice model. In the ground state, spins are organized in two identical quantum loop condensates. Excitations with non-Abelian braiding properties are created by opening loops in each of the copies.

My proposal might open a door for the understanding of the origin of topological states of matter and for the experimental realization of non-Abelian anyons in the laboratory.



[1] B. Paredes, Physical Review B **86**, (2012) 155122.

Jueves 23, 16:40 (invitada)

Electrostatic control of the d_{x2-y2}-d_{3z2-r2} gap and orbital ordering in non-cubic crystals

Pablo García-Fernández[1*], María Teresa Barriuso[2], Juan María García-Lastra[3], Miguel Moreno[1], and José Antonio Aramburu[1]

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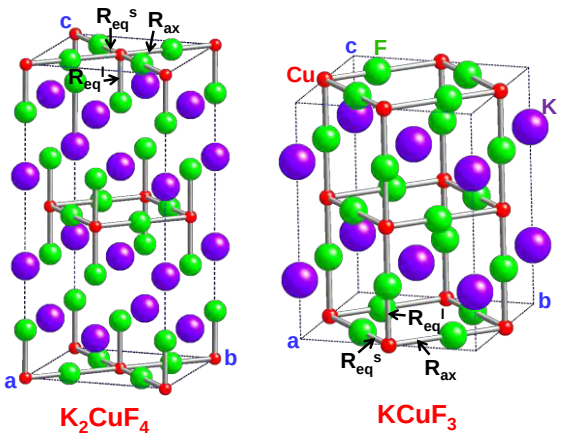
[3]Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Insulating layered compounds containing $3d^9$ Cu^{2+}, Ag^{2+} or Mn^{3+} ions have been widely investigated because of their unique structural, optical, electrical and magnetic properties. However, much more theoretical and experimental work is required in order to understand microscopically many properties, for example, the high-temperature superconductivity. In this sense, different authors have suggested that the transition temperature, T_c, is directly related to the magnitude of the d_{x2-y2}-d_{3z2-r2} splitting, Δ. It is widely assumed that the gap, Δ, in fluorides and oxides containing tetragonal Cu^{2+} or Ag^{2+} complexes directly reflects the tetragonal distortion in the MX_6 complex (M = d^9 ion; X = F^-, O^{2-}). This assumption on that relevant quantity is shown to be not correct through the study of pure K_2CuF_4, $KCuF_3$ and Cu^{2+}-doped $KZnF_3$ and K_2ZnF_4 model compounds [1]. Indeed ab initio calculations prove that Δ in these insulating materials also depends on the internal electric field created by the rest of lattice ions on active electrons confined in a given CuF_6^{4-} complex. Moreover, we show that this internal field over each magnetic complex is also the driving force behind orbital ordering in systems where symmetry-allowed orbital degeneracy is not permitted, where the usual Kugel-Khomskii and Jahn-Teller models are not strictly valid. In order to illustrate the model we focus on K_2CuF_4 and La_2CuO_4 crystals having very similar electronic structure but with contrasting orbital orderings, antiferrodistortive and ferrodistortive, respectively. In a first step we show how the holes in the oxide/fluoride are *completely* driven to the x^2-y^2/$3z^2$-r^2 orbitals. In a second step we demonstrate that the fluoride in this state is frustrated and distorts to the experimental antiferrodistortive state. Moreover, we provide ample data supporting that the model can be applied to many systems allowing the prediction in a simple way of the most stable orbital-ordering pattern.



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Jueves 23, 17:00

A model superspin-glass: random-close-packed maghemite nanoparticles

José A. De Toro[1,*] Su Seong Lee,[2] Peter S. Normile,[1] Pablo Muñiz,[1] Roland Mathieu,[3] Per Nordblad[3], and José M. Riveiro[1]

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A simple single-phase material, a random-close-packed (volume fraction ≈ 67%) ensemble of highly monodisperse *bare* maghemite (γ-Fe_2O_3) nanoparticles, is shown to exhibit ideal *super*spin-glass behaviour (mimicking that of model spin-glasses), namely, an unprecedentedly sharp onset of the absorption component of the ac susceptibility, narrow *memory* dips in the zero-field-cooled magnetization (Figure 1) and a spin-glass characteristic field-dependence of the magnetic susceptibility [1]. In addition, the critical exponents characterizing the phase transition are closer to those measured in spin-glasses than to those reported in particle systems [2]. This ideal behaviour is attributed to the remarkably narrow dispersion in particle size and to the highly dense and spatially homogeneous configuration ensured by the random close-packed arrangement.

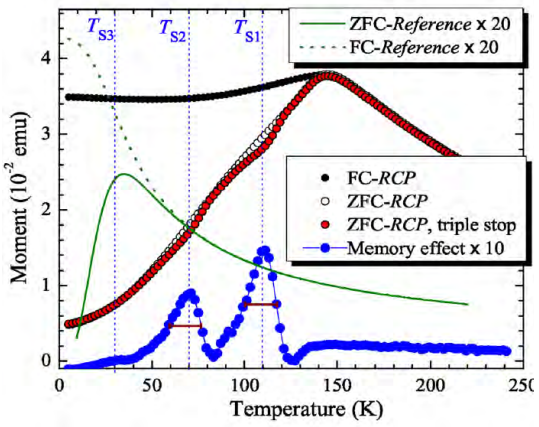

Fig 1. Thermal dependence of the magnetization and memory effect. The FC and ZFC magnetization curves were measured in an applied field of H = 5 Oe in the reference (magnetically diluted) and random-close-packed (RCP) samples. The ZFC curve measured in the RCP sample after 4 h stops at the indicated temperatures (vertical lines) during the cooling is also shown (red symbols). The (scaled) difference between the ZFC curves measured in the RCP sample (blue symbols and guide to the eye) is the memory effect.

Despite the close contact of the *bare* maghemite particles enabling superexchange interactions, the system's freezing temper ture hardly deviates from the value expected exclusively from dipolar interactions. This assertion has been made possible by the comparison between differently concentrated random systems of identical maghemite particles (8 nm in diameter) [3], where the concentration was controlled through the thickness of a silica shell. The random-close-packed ensemble of bare ferrimagnetic particles is argued to constitute the closest nanoparticle analogue to a conventional (atomic) magnetic state found to date.

Preliminary results in a similarly packed system of maghemite particles, but 11 nm in diameter, with a freezing temperature above room temperature, will also be presented.

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[2] R. Mathieu, J. A. De Toro, D. Salazar *et al*., EPL **102** (2013) 67002.
[3] J. A. De Toro, P. S. Normile, S. S. Lee *et al*. , J. Phys. Chem. C **117** (2013), 10213.

Jueves 23, 17:20

Quantum forces in Solids

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Forces of quantum nature are known in physics. One example is a Casimir force between two surfaces in a close proximity to each other. It is caused by the quantization of the fields in the space between the surfaces. In this talk we will discuss the force of a purely quantum origin of another kind: The force that is pertinent to the two-state systems. They correspond to a situation when the lowest energy doublet is separated from the rest of the spectrum by a large gap, making only that doublet relevant in low-energy experiments.

Two-state systems may exhibit mechanical forces of purely quantum origin that have no counterpart in classical physics. We show that such forces must exist in molecular magnets (toy model) due to quantum tunneling between classically degenerate magnetic states. They can be observed in the presence of a microwave field when the magnet is placed in a static magnetic field with a gradient. At low temperature the force is proportional to the tunnel splitting and it disappears on raising the temperature. High magnitude of such forces should make them detectable by micromechanical measurements.

Jueves 23, 17:40

Control of single-spin magnetic anisotropy by exchange coupling

M. R. Calvo [1,#,*], J. C. Oberg[1,2], F. Delgado[3], M. Moro[4,5], D. Serrate[4,5], D. Jacob[6], J. Fernández-Rossier[3], C. F. Hirjibehedin[1,2,7]

[1]*London Center for Nanotechnology, University College London (UCL), London, UK*
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[4]*Instituto de Nanociencia de Aragón , Universidad de Zaragoza, Zaragoza, Spain*
[5]*Departamento de Física de la Materia Condensada , Universidad de Zaragoza, Zaragoza, Spain*
[6]*Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany*
[7]*Department of Chemistry, UCL, London, UK*
[#]*present address: Deparment of Physics, Stanford University, Stanford, USA*

The properties of quantum systems interacting with their environment can be strongly affected by this interaction. While this can lead to unwanted consequences, such as causing decoherence in qubits, it can be also exploited as a probe of the environment, as for example in the case of magnetic resonance imaging.

Depositing magnetic atoms on a thin insulator over a metallic surface has proven to be a successful strategy to study the properties of single atomic spins by Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) [1]. The case of cobalt in copper nitride is of particular interest, its spin ground state is Kondo screened due to exchange coupling to the electronic bath on the substrate [2]. However, the implications of this interaction for the higher spin excitations have not been yet explored.

Here we show that varying the exchange coupling to a nearby conducting electrode can dr m tic lly modify spin's excit tion energy which is determined by the magnetocrystalline anisotropy. Using STM and STS, we observe dramatic variations, as large as a factor of two, in the spin excitation energies of individual Co atoms at different locations on a saturated copper nitride surface as the strength of the spin's coupling to the surrounding electronic b th changes [3]. These observations, combined with calculations, show that exchange coupling can dramatically modify the magnetic anisotropy of a single spin.

This system constitutes one of the few cases in which the energy levels of a quantum system interacting with its environment can be controllably and observably renormalized. Furthermore, we demonstrate that the magnetocrystalline anisotropy, a property normally determined by the local structure around a spin, can be electronically tuned. These effects may play a significant role in the development of spintronic devices in which an individual magnetic atom or molecule is coupled to conducting leads.

[1] C. F. Hirjibehedin *et al*. Science **317**, (2007) 1199
[2] A. F. Otte *et al*. Nature Physics **4**, (2008) 847
[3] J. C. Oberg, M. R. Calvo *et al*. Accepted for publication in Nature Nanotechnology.

ORALES

Sesión 5: - Propiedades ópticas,materiales y dispositivos fotónicos, semiconductores

Viernes 24, 10:00 (invitada)

Engineering quantum light sources through frequency filtering

E. del Valle

Universidad Autónoma de Madrid, Física Teórica de la Materia Condensada, Cantoblanco 28049, Spain

I present our theory on frequency filtered and time-resolved N-photon correlations [1]. These are an extension of the standard Nth order temporal correlation functions (related to the probability of emission of N photons at different times), to include the frequency domain [2,3], as shown in Fig. 1.

With our powerful formalism, we are able to investigate the statistical properties of selected parts in the spectrum of emission of any system (such as quantum dots or quantum dots in a microcavity), unveiling a rich landscape of quantum correlations which allows us to engineer sources of different types of quantum light: single photons [4], high purity N-photon states [5], polarization-entangled photon pairs [6], frequency-entangled photon pairs [7], cascaded pairs of photons with record-breaking Cauchy–Schwarz-inequality violation [8], etc.

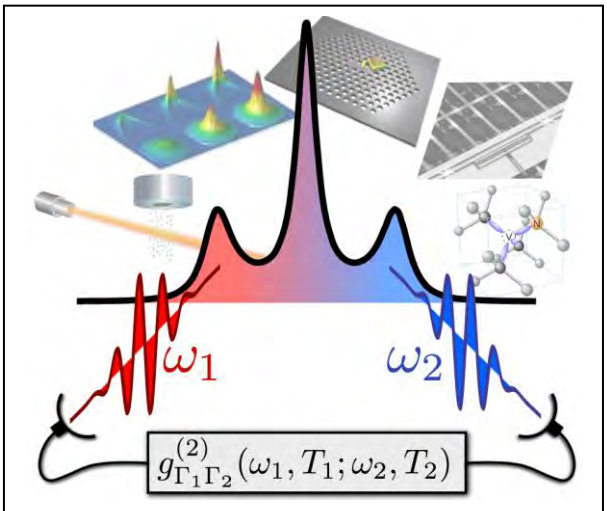

Fig 1. Example of a frequency- and time-resolved 2-photon correlations measurement, extracted from the side bands of the Mollow triplet, the PL lineshape appearing in resonance fluorescence (a qubit scattering light from a laser).

[1] E. del Valle *et al.*, Phys. Rev. Lett. **109**, 183601 (2012).
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[3] K. Joosten & G. Nienhuis, J. Opt. B **2**, 158 (2000); G. Bel & F.L.H. Brown, Phys. Rev. Lett. **102**, 018303 (2009).
[4] A. Gonzalez-Tudela et al., New J. Phys **15**, 033036 (2013).
[5] C. Sánchez-Muñoz *et al.*. arXiv:1306.1578.
[6] E. del Valle, New J. Phys. **15**, 025019 (2013).
[7] E. del Valle *et al.*. In preparation.
[8] C. Sánchez-Muñoz *et al.*. In preparation.

Viernes 24, 10:20 (invitada)

Enhancement of the nonlinear response and the spontaneous emission of Nd^{3+} doped $LiNbO_3$ by silver nanoparticles arrays

P. Molina*, E. Yraola, J. L. Plaza, C. de las Heras, M. O Ramírez and L.E. Bausá

Dept. Física de Materiales and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, 28049-Madrid, Spain

Plasmonic nanostructures are currently the subject of intensive fundamental and technological studies intended to improve the performances of existing optical and optoelectronic devices. These applications relay in the unique features of plasmonic nanostructures to strongly concentrate electromagnetic fields in the vicinity of their physical boundaries, enhancing the interactions between optical species (atoms, QDs, organic fluorophores, etc) and far-field light. Nevertheless, the interaction of photons with the conduction electrons of a plasmonic material involves optical losses, which for optical frequencies can be significant, limiting the final performance of the devices. Probably, the most promising strategy to mitigate these losses is the association of metallic nanostructures with different laser gain media, giving rise to successful configurations such as nanolasers or lasing-spasers in which loss-free operation can be envisage.

In this work, periodic arrays of Ag nanoparticles (NPs) are photochemically self-assembled on the ferroelectric domain walls present in a Nd^{3+} doped periodically poled $LiNbO_3$ (PPLN) laser crystals. The alternative metallic NPs configurations can be exploited to selectively enhance a particular Stark transition of Nd^{3+} ions. As a result, directional enhancement of a single Stark line, particularly the π-polarized Nd^{3+} laser line at 1.08 μm, is demonstrated in a material of technological interest such as $LiNbO_3$. The enhancement of the spontaneous emission of Nd^{3+} Stark laser transition exhibits a micrometric spatial periodicity provided by the formation of metallic Ag NPs chain-like arrangements on the surface of the PPLN structure. Additionally, taking advantage of the nonlinear character of $LiNbO_3$ crystal, the interaction between the Ag NPs and the second harmonic signal is also studied to demonstrate a remarkable intensification of the quadratic nonlinear response of the PPLN, in a factor of 20, which takes place with the periodicity of the metallic arrays.

The results can be extended to the 2D case to exploit the nonlinear properties of different types of alternating ferroelectric domain structures on active materials, which constitutes an alternative approach in the search for sub-micrometer wavelength lasers or gain-enhanced nanoplasmonic metamaterials.

Viernes 23, 10:40 (invitada)

A new bottom-up methodology to produce silicon layers with a closed porosity nanostructure and reduced refractive index

V.Godinho*

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Porous silicon is still nowadays one of the most actively researched materials for diverse applications such as sensors, photonic devices, microelectronics and solar energy conversion [1-4]. Being fully compatible with the established microelectronic technology, one of the most attr cting fe tures of porous silicon is its ~~"~~made to order" refr ctive index.

Porous silicon has been produced by a variety of approaches, but it is most commonly prepared by electrochemical etching in HF based solutions. Recently, we presented for the first time the possibility to produce amorphous porous silicon coatings (a-pSi) with closed porosity by magnetron sputtering. Our approach is a new bottom-up methodology to produce porous silicon coatings with closed and controlled porosity by magnetron sputtering [5]. It is shown how the use of He as process gas gives rise to a singular microstructure of closed pores, filled with the deposition g s ligned on the co tings' growing direction. High resolution analytical electron microscopy techniques are employed here to characterize the coatings porosity and evaluate the gas inside the pores, allowing an estimation of its pressure.

Also the mechanisms beyond the formation of the closed porosity in these coatings need to be investigated. Do the close pores form during deposition trapping the deposition gas or are they consequence of post deposition processes? How is the microstructure changing when another inert gas as Argon is used? To draw light into these questions, experimental results were compared with theoretical models.

This new approach introduces many advantages over the traditional procedures, especially supported on the fact that magnetron sputtering is a very versatile deposition technique that allows not only to deposit on large scale but also on cheap and/or flexible substrates. The introduction of porosity significantly reduces the refractive index of the coatings as compared to the dense ones. The achievement of closed porosity was desired to improve the chemical and mechanical stability as compared to materials previously prepared by etching methodologies with open porosity. Moreover, we demonstrated the possibility of tailoring the microstructure in function of the deposition conditions and thus the properties of the coatings, and the feasibility of producing multilayers alternating different structures: closed pores, dense or columnar structures.

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[2] H. Jin, G.L. Liu, Nanotechnology, 23 (2012) 125202.
[3] K. Zhang, J.-H. Seo, W. Zhou, Z. Ma, Journal of Physics D: Applied Physics, 45 (2012) 143001.
[4] P. Spinelli, M.A. Verschuuren, A. Polman, Nat Commun, 3 (2012) 692.
[5] V. Godinho, J. Caballero-Hernández, D. Jamon, T.C. Rojas, R. Schierholz, J. García-López, F.J. Ferrer, A. Fernández, Nanotechnology, 24 (2013) 275604.

Viernes 23, 11:40

Semiconducting polymers with a high figure of merit

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Materials Science Institute, University of Valencia PO Box 22085, 46071 Valencia, Spain

Conducting polymers have attracted considerable attention in the last years in electronic applications. Conducting polymers like polythiophene, polypyrrol and polyaniline have been the most used since the initial discovery of doped polyacetylene in the late 1970s [1]. These polymers are semiconductors that provide a reasonable electronic conductivity after doping with suitable dopants. They have been extensively studied for their numerous applications like light-emitting diodes, sensors, photovoltaic cells and thermoelectric devices. In these applications, it is important to control the electronic properties of the material. Particularly, in poly(3,4-ethylenedioxythiophene), PEDOT, the doping level is easy to control by chemical reduction. This work focuses on the study of the thermoelectric properties such as electric conductivity, Seebeck coefficient and thermal conductivity of PEDOT films with several counter-ions as a function of the reduction level. This is a novel route to increases the thermoelectric efficiency, generally measured by the figure of merit ($ZT=\sigma\ ^{2}T/\kappa$). PEDOT films have been synthesized by electro-polymerization in an electrochemical cell and the chemical reduction was carried out keeping the PEDOT film in contact with hydrazine vapor. Very high ZT values have been obtained, around of ZT~0.22, at room temperature.

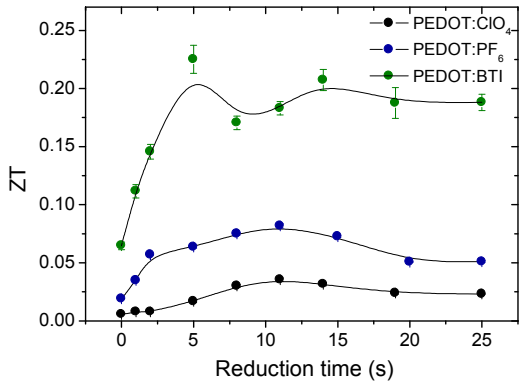

Fig 1. ZT values of PEDOT with several counter-ions as a function of reduction time at room temperature.

[1] H. Shirakawa, E. J. Louis, A. G. MacDiarmid, C.K. Chiang and A.J. Heeger. Journal of the Chemical Society, Chemical Communications **16**, (1977) 578.

Viernes 23, 12:00

Propagation of polariton waves and polariton wavepackets

David Colas[1], Juan Pablo Restrepo[2], Guillermo Guirales[2], Blanca Silva Fernández[1] and Fabrice P. Laussy[1,*]

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Microcavity polaritons are versatile quasi-2D bosonic particles that arise from the strong coupling of light (cavity photons) and matter (quantum well excitons). As a result, they combine properties such as a very high degree of coherence and strong nonlinearities [1]. They are also highly dissipative systems, allowing for a constant monitoring of their dynamics due to the continuous photon leakage from the structure. From the viewpoint of Bose condensates, they have opened a new door on the physics of strongly correlated systems [2]. Thanks to the great experimental freedom in the excitation of the system—in particular with possibilities to impart momentum (linear and/or angular), to excite various modes of the system by pulse shaping or to do ultra-fast imaging of the dynamics through interferometry—these systems are an ideal laboratory to investigate the coherent fluid dynamics in a variety of contexts, such as propagation of bullets [3], superfluidity [4] and the dynamics of vortices [5] (see [6] for a review).

In this talk, an overview of the state of the art will be given and the propagation of polariton fluids shown to be extremely peculiar even in the linear regime of excitation (low pumping), thanks to the peculiar dispersion of the particles [7]. We will describe in particular the free and scattered propagation of localised packets in various geometries, and how the counterpart of Airy beams—too heavy to be propagated by polaritons—can be realized in such structures [8]. In the nonlinear regime, we will show how this blossoms into a dynamics of unsupected beauty, such as the formation of a quantum backjet, that sucks all the fluid and appears to freeze in time [9].

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[5] "*Persistent currents and quantized vortices in a polariton superfluid*", D. Sanvitto et al. Nat. Phys. 6, 527 (2010).
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[7] "*Quantum Dynamics of Polariton Condensates*", F.P. Laussy, Chap. 1 in the previous reference.
[8] "*Propagation of polariton waves and polariton wavepackets*" D. Col s et l. unpublished.
[9] "*Backjet, shock waves and ring solitons in the quantum pond of a polariton superfluid*", L. Dominici et al. arXiv:1309.3083 (2013)

POSTERS

Graphene on Pt(111): Low Temperature Noncontact Atomic Force Microscopy measurements and First-Principles Calculations

B. de la Torre[1], M.E. Ellner[2,*], P. Pou[2,3], N. Nicoara[1,4], R. Pérez[2,3], J. M. Gómez-Rodríguez[1,3]

[1]*Dept. de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain*
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The epitaxial growth of graphene on metals is currently an active field of research[1)]. Scanning probe techniques have revealed as fundamental tools for the analysis of the atomic and electronic structure of graphene. However, the origin of atomic contrast in carbon based systems is still a challenging question[2)]. Graphene on Pt(111) is of utmost interest due to the low interaction of its pristine surface with the metal[3)]. In this work, for the first time, noncontact atomic force microscopy measurements with atomic resolution at low temperature (5K) and UHV of graphene/Pt(111) are reported. The origin of the atomic contrast, as well as the occurrence of contrast inversions, are rationalized in terms of ab-initio DFT calculations, based on the OpenMX code, for a G_{6x6} Moiré and a reactive Pt tip. For this tip, the short-range interactions are responsible for the atomic contrast. Due to the electronic density dependence of the Pauli interaction, greater forces on the carbon atoms in the attractive regime and a crossing of the top/hollow force curves at closer distances is obtained. On the other hand, the Van der Waals force promotes a background of attractive interaction which can be measured experimentally. Many methods for including dispersion interactions into DFT have been developed, including semi-empirical corrections[4)] and exchange-correlation functionals that include van der Waals interactions[5)] and we experiment with them in order to determine which one reproduces more accurately the experiments.

[1] A. J. Martínez-Galera, et al. Nano Lett. 11, 3576 (2011).
[2] M. Ondráček, et. al. Phys Rev Lett. 106, 176101 (2011).
[3] M. M. Ugeda, et al. Phys Rev Lett. 107, 116803 (2011).
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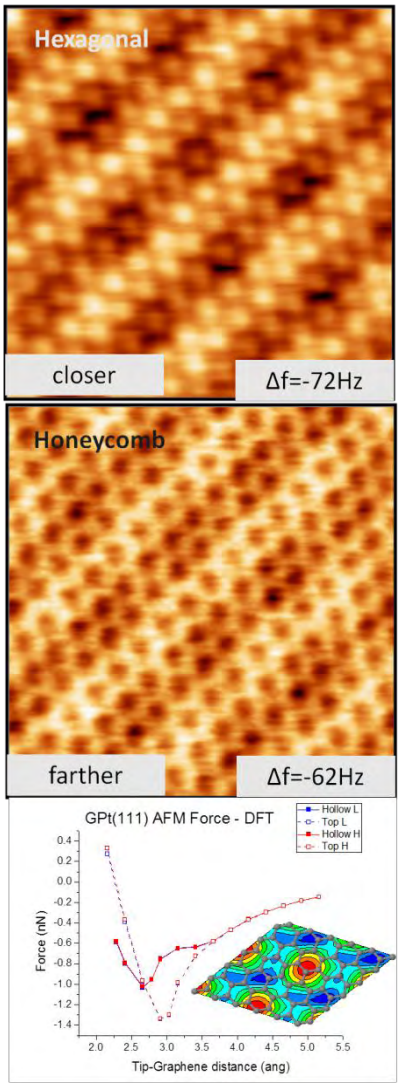

Fig 1: Top: experimental moiré pattern. Bottom: DFT calculations

Temperature-induced spin density wave in a magnetically doped topological insulator Bi_2Se_3

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Topological Insulators (TIs) are a newly discovered type of systems which are insulating in the bulk and are characterized by the existence of a robust helical gapless Dirac 2D electron system at their surface.

We study the magnetics properties of Bi2Se3 doped with isoelectronic magnetic impurities. We analyze the coupling of the non-uniform magnetic phase with the Dirac electronic system that occurs at the surface of the topological insulator.

Ab initio study of Z_2 topological phases in perovskite (111) $(SrTiO_3)_7/(SrIrO_3)_2$ and $(KTaO_3)_7/(KPtO_3)_2$ multilayers

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The quest for new topological insulators has been sparking in recent times. Oxides provide a promising platform due to their chemical stability and ease of nanostructurization. Among them, perovskite oxide bilayers grown along the (111) direction have been shown [1] to develop topological phases depending on the filling of the d shell and the strengh of the spin orbit coupling (SOC), whose gap is developed when a term with trigonal symmetry is turned on.

We have focused [2] on the t^5_{2g} configuration and strong spin-orbit coupling, 5d transition metals. In the strongest SOC regime, the topological phase developed is mathematically equivalent to the Kane Mele model, but with the topological gap opened linearly trough a third order process by the trigonal field felt by the transition metal atoms instead of the usual SOC in graphene. Reducing the SOC drives the system to a phase which is no longer equivalent to the Kane-Mele model, nevertheless being topologically connected to the previous one.

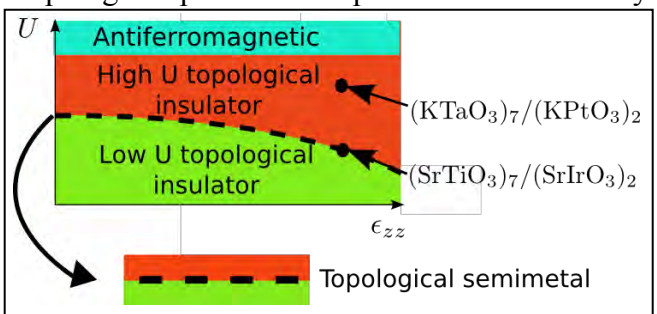

Fig. 1: Phase diagram of the two multilayers for e-e interaction and uniaxial strain, the position of their ground state is shown.

Taking as particular materials the multilayers cited in the title, we performed ab initio DFT calculations and we have calculated the Z2 invariant of the systems, showing that both systems can develop a topological phase in a regime classified as intermediate SOC. Modifying the electron-electron onsite interaction and the uniaxial perpendicular strain, we showed that these systems suffer a transition between two topological insulating regimes, passing through a crossing point where the systems behave as a topological semimetal.

Very much like as in graphene, there is a competition between the topological gap opened by the inversion symmetric trigonal term and the trivial gap opened by the sublattice asymmetry. We show that the behaviour of the gap is the one expected from the Kane Mele model as the structure is driven away from the symmetric point.

Finally, we determined that the ground state of the systems would be a topological semimetal for the Ir-based and a topological insulator in the high-U regime for the Pt-based multilayer. Also, we found that both systems would remain non magnetic and their structure would be stable against inversion symmetry perturbations, both necessary conditions to develop topologically-protected protected gapless edge states.

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[2] J. L. Lado, V. Pardo, and D. Baldomir, Phys. Rev. B **88**, 155119 (2013).

Modeling deformation of graphite layers using molecular dynamics

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The interaction of a scanning tunneling microscope (STM) tip with a graphite surface is modeled using molecular dynamics. An upward force, emulating an electrostatic force due to the STM tip, is applied on the first graphite layer. Simulations are performed using the molecular dynamics code LAMMPS [1] with the AIREBO interatomic potential [2]. The initial configuration, with 28800 atoms, consists of a step on the top surface that ends in a zig-zag configuration or an arm-chair configuration. A force is applied at the edge of the step, in a 5 A semicircle located in the center of the simulation box, as shown in figure 1.

We have performed simulations at room temperature for different values of the force applied in order to obtain the minimum value of the force needed to, first, exfoliate this layer and second to break it. In those cases where breaking occurs, the preferential direction for breaking is studied as well as the final configuration of this layer. Results are compared with experimental observations of electro-exfoliation with an STM tip.

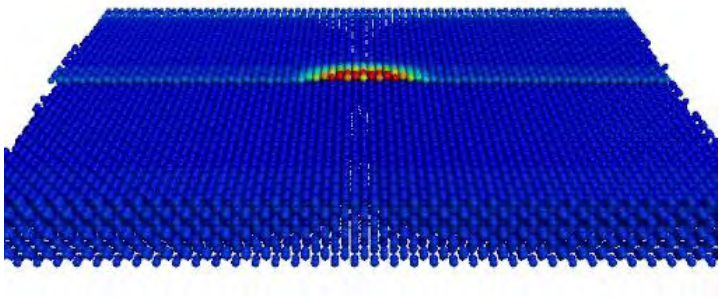

Figure 1: Simulation set up with 28800 atoms in graphite and a step in the top layer. Colors represent the forces applied in the center of the top layer.

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Improving the quality of graphene synthesized by CVD over Ni substrates

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Graphene, an extraordinary two dimensional carbon material with a honeycomb structure, has been the focus of many researches due to its characteristics and its extraordinary mechanical, electronic and optical properties. Chemical Vapor Deposition (CVD) method has been shown to produce large-area and high quality graphene. In CVD, Ni and Cu are normally used as substrates although other transition metals are also used, but less frequently [1].

In order to improve the quality of the graphene layers, the CVD method using Ni substrates has been optimized. Thus, a homemade software was designed in order to analyze the graphene quality, focusing in the image of the sample obtaining using optical microscopy. This software allows know the percentage of each type of graphene presents in the deposited graphene sheet. Depending of the obtained percentage, the software assigned a number between 1 and 1000 which allow quantify the quality of the sample, obtaining a number between 0 and 10 if the most of the sample is multilayer graphene or few-layer graphene, between 10 and 100 if the most of the sample is bilayer graphene and between 100 and 1000 if the most of the sample is monolayer graphene [2].

The objective of this work was to improve the homogeneity and thus, the quality of the synthesized graphene over Ni, obtaining more percentage of monolayer graphene while the synthesis parameters of the CVD-grown graphene were optimized.

Raman spectroscopy were used to analyzed the obtained graphene due to it is considered the most potential method for non-destructive and quick structural characterization of graphene and graphite materials [3].

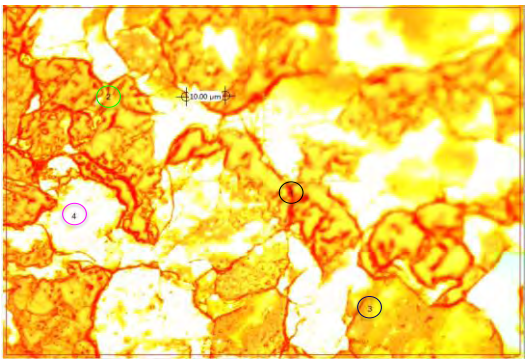

Fig 1. Optical Microscopy of graphene synthesized over Ni showing the analyzed points.

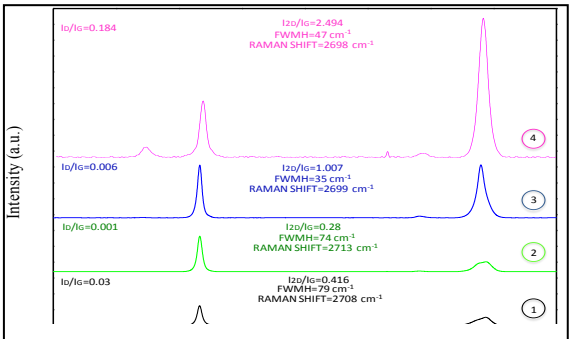

Fig 2. Raman Spectroscopy of the points showed in Fig. 1 and main Raman parameters

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Canted magnetism end edge transport in tunable quantum Hall phases in graphene

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Motivated by recent experimental results [1] we study theoretically the quantum Hall effect in graphene in the presence of strong in plane magnetic field considering short range electron electron interactions. The experiments show a variety of phase transitions that change the bulk spin order order between different states, including antiferromagnetic (AF), ferromagnetic (FM) canted antiferromagnetic (CAF) and non magnetic, resulting in dramatically different edge states that control the conductivity. Here we model the non-trivial phase diagram of this system using a Hubbard model for a wide ribbon in a non-collinear mean field approximation. Our theory [2] is able to account for the main experimental findings and provides a comprehensive phase diagram with at least 5 different electronic phases: AF, FM, CAF, ferrimagnetic phase and non magnetic. Specifically, our model describes the presence of counter-propagating spin-filtered edge states in the FM phase at half filling, as well as a fully polarized single edge channel when the FM phase is doped into a ferrimagnetic phase with an electron-hole gap.

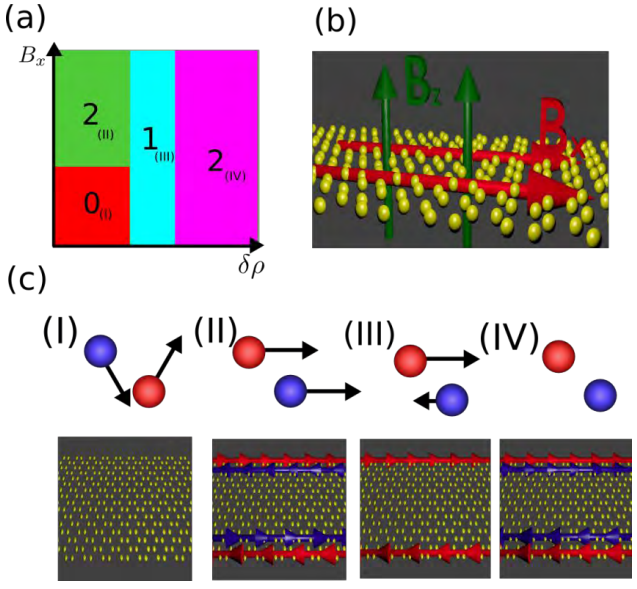

Fig. 1: (a) Phase diagram of quantum conductances as a function of the inplane magnetic field and doping, (b) scheme of the experimental setup, (c) magnetic orderings and edge chanels of each phase

[1] A. F. Young, J. D. Sanchez-Yamagishi, B. Hunt, S. H. Choi, K. Watanabe, T. Taniguchi, R. C. Ashoori, P. Jarillo-Herrero, arXiv:1307.5104
[2] J. L. Lado and J. Fernández-Rossier, manuscript in preparation

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Electrostatic Manipulation of Graphene on Graphite

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Here we report the use of a Scanning Tunneling Microscope (STM) under ambient conditions to study the controlled exfoliation of the last layer of a graphite surface when an electrostatic force is applied from a STM tip.

In this project we have focused on the study of two parameters: the applied voltage needed to compensate the interlayer attractive force and the one needed to break atomic bonds to produce folded structures. Additionally, we have studied the influence of edge structure in the breaking geometry.

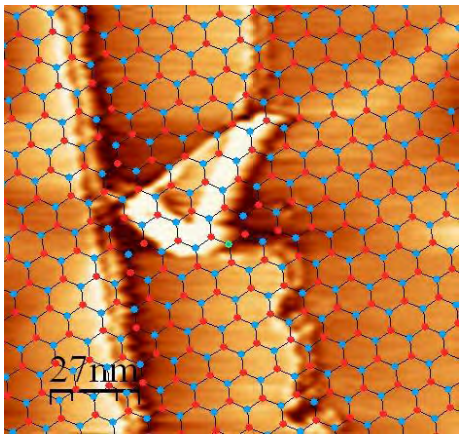

Fig 1. Graphite terrace after voltage ramp with edge structure.

References:

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Molecular dynamics and TEM image simulations of ion implantation in Fe thin films

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[1] *Dept. Física Aplicada, Facultad de Ciencias, Fase II, Universidad de Alicante, Alicante, E-03690, Spain*
[2]*Ecole Polytechnique Fédérale de Lausanne (EPFL), Centre de Recherches en Physique des Plasmas, Association Euratom-Confédération Suisse, 5232 Villigen PSI, Switzerland*

Ion implantation experiments are being used extensively to understand damage production and damage evolution due to irradiation. These experiments aim towards gathering basic understanding of these processes to be able to build a predictive model for neutron irradiation. In order to build such predictive model it is important to understand the basic differences between the initial damage produced under ion implantation and neutron irradiation. In this work we present molecular dynamics simulations of Fe thin films (up to 100nm), corresponding to 20 million atoms specimens, implanted with Fe ions with energies between 50keV and 150keV. Two different interatomic potentials have been used, as well as different impact angles and at 0 K and RT. The damage produced is analyzed in detail in terms of total defects produced and cluster size distribution and type. The results are compared to bulk cascades for energies of 50keV and 100keV. Significant differences are observed, from the total number of defects to the cluster size and character, due to the presence of surfaces. For example, large vacancy clusters are produced under ion implantation more frequently than in the bulk. They occur near the surfaces. In addition it seems that the largest defect clusters close to surfaces are vacancy in nature and have a Burgers vector <100>, while elsewhere and for bulk specimens they are only ½<111> and of interstitial nature. In order to compare directly to experimental observations, TEM image simulations have been performed.

Valence Band Circular Dichroism from a Single Ru(0001) Terrace

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Dichroism in material science has been often used to gain insight of properties of surfaces. In particular, magnetic circular dichroism at an x-ray absorption edge is well known as a technique that allows the determination of magnetic properties of films and surfaces. But not only magnetic surfaces show dichroism. In particular, in photoemission, dichroism can arise if the incoming light direction, the crystalographic axes and the emission direction form a chiral triplet, i.e. application of a symmetry operation of the crystal does not produce the same experimental configuration [1]. This dichroism in the absence of either sample chirality or magnetism has been observed in two different configurations, either with normal incidence and off-normal emission [2], or with off-normal incidence and normal emission [3].

We will present our first measurements on the dichroism at the valence band, close to the Fermi level, of Ru(0001). We use the combined low-energy and photoemission electron microscope of the CIRCE beamline of the Alba synchrotron. Ru(0001) presents an additional complication: while the bulk material has six-fold symmetry, a given surface termination presents three-fold symmetry. The symmetry of the surface might be observable in photoemission if any surface features such as surface states are available. The symmetry of each terrace is readily observable by means of dark field contrast: if a low-energy electron image [4] is acquired at the proper energy with a first order diffracted spot, terraces are imaged dark and bright upon crossing atomic steps [5]. In this work we will present our results imaging the distribution of photoelectrons from areas with mostly a given terrace type on a Ru(0001) single crystal close to the Fermi level employing circular and linearly polarized x-rays.

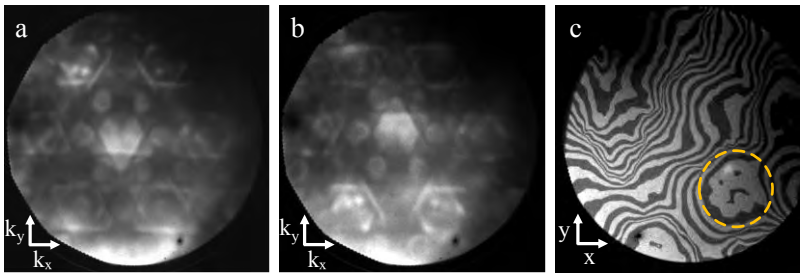

Fig.1. Valence band distribution of electrons from a single Ru(0001) terrace, acquired with left (a) and right (b) x-ray polarization. The x-ray beam is coming along the x-axis. The photon energy is 140 eV and the kinetic energy is 136.25 eV. (c) Dark field image of the Ru(0001) surface. The dashed circle indicates the terrace where the previous photoemission electron images were taken. The kinetic energy is 33.25 eV.

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Formación de un subóxido epitaxial mediante bombardeo iónico sobre la superficie (110) del TiO_2-rutilo.

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Existen numerosos estudios sobre la manera en que se ven alteradas las propiedades de la superficie de TiO_2(110) cuando es modificada mediante bajas dosis de bombardeo iónico. Sin embargo, hasta el momento no se ha estudiado a fondo cómo se ve modificada la estructura de esta superficie bajo altas dosis de bombardeo iónico.

En este trabajo, se utilizan distintas técnicas para caracterizar la superficie modificada, tanto en cuanto a su estructura como a su composición química.

Mediante técnicas de espectroscopia de electrones Auger (AES) y espectroscopia de fotoemisión de rayos X (XPS), se ha hecho un seguimiento de la evolución química a distintas dosis de bombardeo, confirmando que éste crea vacantes de oxígeno y hace por tanto que los cationes de titanio reduzcan su valencia.

Basándonos en técnicas de difracción de superficies, como es la difracción de electrones de baja energía (LEED), realizada en nuestro laboratorio, y la difracción superficial de rayos X (SXRD), realizada en la línea SpLine del Sincrotrón ESRF, identificamos una nueva estructura en la superficie modificada, que se corresponde, en las tres direcciones del espacio, con la celda unidad del TiO(001), rotada 45º dentro del plano con respecto a la del rutilo. El grosor de esta capa es bastante mayor que la profundidad alcanzada por el daño directo de los iones, por lo que se deduce que la difusión juega un papel importante en este proceso.

Fig 1. Representación en el espacio recíproco (L=0.3) de la celda unidad del TiO, obtenida mediante SXRD.

Hasta el momento no se conocen casos de la inducción de una nueva estructura cristalina mediante bombardeo iónico. Sin embargo, en este trabajo se muestra que, bajo condiciones de alto flujo y altas dosis, el bombardeo iónico de baja energía sobre la superficie TiO_2(110) produce la formación de una capa cristalina pseudoepitaxial con la estructura de un subóxido: TiO(001).

Stoichiometry and structure control of iron-oxide ultra-thin film

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Iron oxides are promising materials because their physical and chemical properties can be tailored by changing their stoichiometry and structure. Binary iron oxides vary their electrical properties from conductors, like magnetite, to insulators, like maghemite, and their magnetic properties range from ferrimagnets to antiferromagnets. For these reasons, understanding the role of the experimental parameters during their synthesis is a fundamental issue in iron oxides research, with implications in different fields as corrosion, medicine, catalysis and spintronics [2-4].

In the present work we aim at understanding the growth details of different iron oxide ultra-thin films by varying the experimental parameters. The iron oxide were grown on a Ru(0001) single crystal using oxygen-assisted molecular beam epitaxy. The nucleation and growth of the iron oxide films have been observed in real time by low-energy electron microscopy (LEEM), and the films have been characterized using selected-area low-energy electron diffraction (LEED).

First, the influence of the oxygen pressure on the growth mechanism will be presented. We propose that, during the initial stages, the film thickness is controlled by the concentration of oxygen absorbed on Ru(0001)[5]. Second, the influence of the iron dosing rate on the iron oxide ultra-thin film will be reported. We finally discuss the possibility to control the stoichiometry and structure of the ultra-thin film by choosing accurately the iron deposition rate.

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Contribution of polar nanorregions to the giant flexoelectricity of relaxor ferroelectrics.

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We have studied the bending-induced polarization of single crystal relaxor ferroelectrics close to a morphotropic phase boundary. Anomalously large flexoelectric and flexocoupling coefficients were registered, with values well in excess (up to10 times bigger) than theoretical expectations based on Kogan's theory [1] below critical temperature. The temperature dependence of the effective flexoelectric coefficients shows that this anomalous enhancement persists in the temperatures up to T*~250^{o}C, above which the values fall back in line with theoretical expectation for pure flexoelectricity. Cross-correlation between flexoelectric and elastic measurements indicates that the anomalous enhancement of bending-induced polarization is caused by the flexoelectric reorientation of non-percollating polar nanotwins that exist in the temperature range between Tc and T*.

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Orbital reconstructions in transition metal oxide heterostructures

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[1]*Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Catalonia, Spain*
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In transition metal oxides (TMO) strong correlations between electrons in *d* orbitals are at the origin of their diverse fascinating properties. The highly anisotropic and localized character of *d* orbitals and the strong electron-lattice coupling allows for a fine tuning of the occupancy among the different electronic states, eventually leading to a control of their spin and charge [1]. The presence of surfaces/interfaces –and the inherent space-symmetry breaking– as well as epitaxial strain in thin films, are factors that modulate the electron occupancy. Therefore, a deep understanding of how electrons are arranged in *d*-states of TMO as a function of these parameters is fundamental for understanding the origin of the physical and chemical properties.

Here, we will report data on 3d and 4d oxides ($La_{2/3}Sr_{1/3}MnO_3$, $LaNiO_3$ and $SrRuO_3$) and we will show that electronic occupancy at e_g (x^2-y^2; z^2) and t_g(xy, xz, yz) orbitals results from a delicate balance between the symmetry breaking strain and free surface effects, modulate by their spatial extension (3d *vs* 4d). We will also show that capping of the functional layer by dissimilar oxides can also a profound rearrangement of the orbital occupancy that shall be of relevance for the functionalities of TMO heterostructures.

By means of X-ray absorption dichroism measurements (both linear and circular) with synchrotron radiation, we have determined the orbital occupancy of $La_{2/3}Sr_{1/3}MnO_3$, $LaNiO_3$ and $SrRuO_3$ epitaxial thin films, in a wide range of thicknesses, grown on different substrates imposing either compressive or tensile strains. We shall review the role of structural distortions in the orbital polarization and in the metal-oxygen hybridization, as well as newly found special electron occupancies at the bare surfaces of these oxides [2], and the occurrence of orbital reconstructions at the interfaces with other oxides. We will overview the impact of these orbital arrangements on the magnetic and transport properties of these materials and the possibilities for new functionalities for electronic or catalytic applications.

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CO adsorption sites on a strained Pd(111) surface supported on TiO_2(110)

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Supported metal nanoparticles are frequently used as models of heterogeneous catalysts, with behaviour thought to be dependent on the nanoparticle size. Above a certain size it has generally been assumed that the nanoparticle behaves in the same way towards adsorbates as would a semi-infinite crystal. In this work, we examine this proposition using CO adsorption on Pd nanoparticles supported on TiO2(110) combining scanning tunnelling microscopy and DFT calculations[1,2]. The results show that the CO lateral registry differs from the single crystal. This phenomenon arises from a curvature of the nanoparticle that is caused by the underlying substrate step-edges. At a CO coverage of half a monolayer, two types of CO adlayer form in addition to those observed on the native Pd(111) surface [3]. Density functional theory calculations on a c(4 x 2) unit cell and including 2 CO molecules suggest that their formation is driven by curvature-related strain. We have determined the relative stability of different molecular adsorption configurations under both uniform 2D strain and 1D strain (using the bulk Pd Poisson's ratio to take into account the deformation in the normal direction). Our calculations show that sufficiently large strains stabilize bridge-bridge (BB) and top-hollow (TH) configurations and reduce the energy difference with the fcc-hcp (HH) ground state.

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A Theoretical DFT Study of the (√13x√13)R13.9º reconstruction of the fullerene C_{60} on Pt(111) using van der Waals Functionals

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The microscopic understanding of the adsorption of large organic molecules on metallic surfaces has become a very active field of research due to their ability to tune the surface electronic properties and chemical reactivity. In particular, it has been shown that the C_{60} fullerene deposited on Pt(111) has excellent electronic properties with possible applications as a rectifier in molecular electronics. Experimental evidence, based on Surface X-Ray Diffraction, reveal the existence of a reconstruction in this system involving the formation of a vacancy network [1].

In this work, we determine the lowest energy adsorption configurations for C_{60} exploring the complex parameter space spanned by the possible adsorption sites and different molecular orientations. In order to understand the competition between the intermolecular and the molecular substrate interactions, these calculations are performed both in a large 5x5 unit cell –that represents the isolated single molecule limit–, and with the (√13x√13) periodicity identified in the LEED and STM experiments. In these simulations, we include the effect of van der Waals interactions, comparing two different approaches: a semi-empirical method [2] and the recently developed exchange-correlation functionals that include van der Waals corrections [3].

Our detailed study provides an explanation for the contrast evolution as a function of temperature found in recent STM experiments and its relation with the translational and rotational order of the system [4]. Furthermore, we gain insight into the mechanisms involved in the vacancy network formation. We show the relevant role played by intermolecular interactions and propose some stable structures based on vacancy-adatom pairs (figure 1) as the likely candidates for the transition state and final configuration in the C_{60}/Pt(111) system.

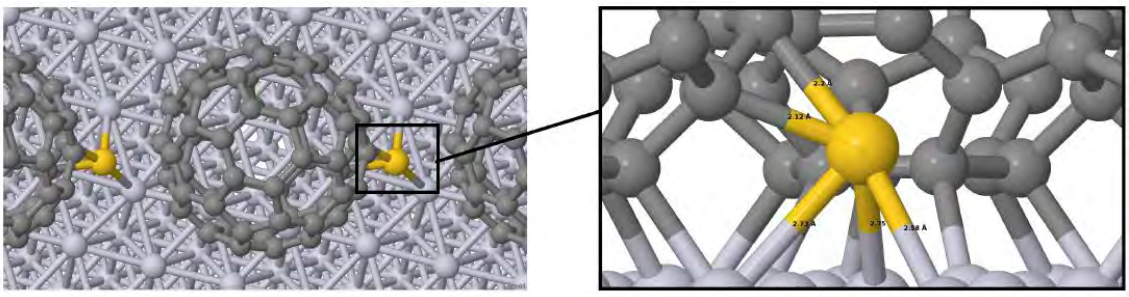

Fig 1: One of the proposed stable structures: The vacancy is right below the molecule and the adatom (in yellow) is located in one hcp-hollow position in the neighborhood of the molecule forming two C-Pt bonds.

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The interaction of two metallic surfaces at the atomic level

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When two metallic electrodes approach each other, a jump in the conductance is observed in some cases. For example, when an Au or Cu nanocontact breaks and the two tips are again brought into contact, a jump to contact is observed [1]. However, when a tip is brought into contact with an adatom on a surface no jump in the conductance is measured [2].

In order to understand this behavior, we have studied this phenomenon in Cu and Au using molecular dynamics with EAM interatomic potentials [3]. Firstly, a nanocontact is stretched until it breaks. The tip so formed is then used to study contact with different surfaces: a flat surface, a flat surface with an adatom and a contact with another tip. Simulations are performed at 4.2K and 8K and for different orientations of the nanocontact, [111], [110] and [100].

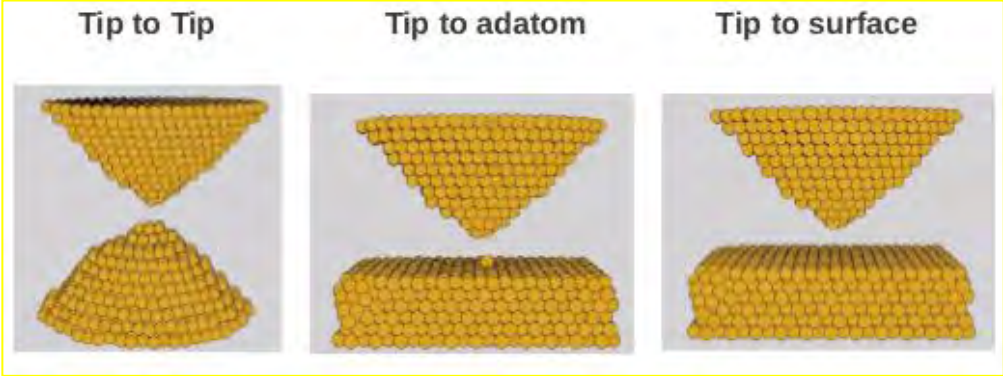

Figure 1: Configurations for tip to tip, tip to adatom and tip to surface contacts.

Figure 1 shows the configuration of a Cu tip and a surface with and without an adatom. The atoms that make contact first are identified in the simulation and the distance between these two atoms is recorded as a function of simulation time (or electrode displacement). In this way we can study the presence of a jump to contact. Simulations show that the shape of the tip determines the presence or absence of a jump to contact. Other materials with different crystallographic structures, such as W and Fe, are also being studied.

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Magnetic Properties of Transition Metal Impurities (Mn, Fe, Co) in MgO

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Motivated by the great interest in MgO based tunnel barriers with large magnetoresistance, we study the impact of magnetic dopants in MgO. Specifically, we consider the case of transition metal impurities (Mn, Fe, Co) replacing Mg atoms. We theoretically analyze the magnetic properties of the $Mg_{31}O_{32}X$ bulk (64 atoms unit cell), where X is a transition metal (Mn, Fe or Co). Calculations based on Density-Functional Theory (DFT) were performed using the projector augmented wave (PAW) and generalized gradient approximation (GGA) exchange-correlation functional as implemented in Quantum Espresso code. We perform DFT calculations and we derive a tight-binding model with the aim of understanding the effects of the transition metals in the magnetic properties of the system. The basis set used to obtain the tight-binding Hamiltonian is provided by the maximally localized Wannier functions (MLWF) generated from the DFT calculations using the Wannier 90 package. Our calculations show that the $Mg_{31}O_{32}X$ has a quantized magnetic moment (S=5/2 for X=Mn, S=2 for X=Fe and S=3/2 for X=Co) localized in the dopants atoms. We also analyze the d level splitting of the flat bands introduced by the transition metal atoms inside the MgO gap.

A multi-orbital single site Anderson model is build using the tight-binding Hamiltonian obtained from DFT and extended to include spin orbit coupling. The exact numerical diagonalization of the Anderson model yields the effective single ion spin Hamiltonian for the transition metals in the cubic environment of the MgO.

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Strong Phonon Energy-Shift In One-Atom Contacts Due Uniaxial Strain

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It is known that contact spectroscopy of bulk gold at cryogenic temperatures exhibit two distinct spectroscopy peaks corresponding to the longitudinal and transversal excitation of bulk phonon modes [1]. On the other hand, atomic chains spectroscopies exhibit only one strong vibrational peak corresponding to excitation of the longitudinal phonon mode [2]. The frequency of these phonon modes show significant sensitivity to strain in the nano/atomic-chain contact in which they are fabricated, and although energy shifts due strain have been strongly investigated for atomic-chains, a full transition from bulk spectroscopy features to atomic chain features, both in strain and compression, has not been investigated.

The present work addresses that transition point, the single atomic contact. Via contact spectroscopy done along both rupture and formation of the 1Go plateau of gold edge-to-edge fabricated single-atomic contacts at 4K, we investigate energy shifts in the spectroscopy phonon peaks. In both compression (formation) and strain (rupture) regimes we observe a point along the plateaus under which the longitudinal and the transversal phonon peaks cross each other, denoting the beginning of the transition from bulk spectroscopy features to atomic-chain spectroscopy signatures. Further results regarding single-atom contact formation geometries, their characteristic spectroscopy features and their correlation to same-trace rupture spectroscopies will also be addressed.

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Unexpected conduction at emerging twin boundaries and dislocations in LSMO thin films

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Transport properties of manganese perovskites depend primarily on band filling, temperature and magnetic field, but in thin film form, they also depend on the existence of lattice distortions [1] and precise structure of the films [2]. In maganite thin films transport properties related to structural distortions have been mainly focused on the role of grain boundaries [3,4]. However, magnetotransport properties can also be drastically affected by the strain misfit caused by the clamping of the film to the substrate [5]. Perovskite manganites have two different mechanisms to accommodate structural strain: stretching or compressing its bond lengths, or by tilting of its oxygen octahedra [6]. The first mechanism usually yield to the formation of dislocations to release the stress of the layer, while by the latter mechanism gives rise to the formation of twin structures which allows the accommodation of strain at a low energy cost [7,8]. The formation of those two strain releasing structures are observed in $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) thin film grown on in $LaAlO_3$ (001)(LAO) and $SrTiO_3$(001) (STO). In this work we report local conductivity measurements over epitaxial LSMO films with presence of twin structures or dislocations along the film. An unexpected enhancement of conductivity along twin boundaries is measured, whereas a decrease of the current is found on the dislocations locations.

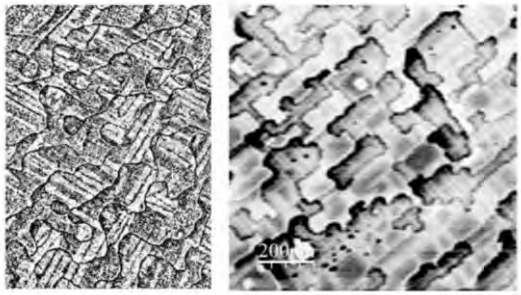

Fig 1. Conducting AFM maps of: 40nm thick LSMO on STO (left) presenting twins due to tensile strain and 3.5 nm thick LSMO film on LAO (right) presenting dislocations due to compressive strain.

CSFM measurements reveal an unexpected local conductive response on the location of strain releasing structures as compared to the rest of the LSMO layer surface. An enhancement of conductivity along twin boundaries is measured, whereas a decrease of the current is found on the dislocations locations.

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Control of block-copolymer nanostructures in thin films: geometrical configuration and magnetic nanoparticles

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In recent years block-copolymers have become an important field of interest due to their tendency to segregation in different phases over space and therefore to self-organization properties on surfaces, making them capable of reproduce structure patterns of a material over great areas [1]. Original studies of basic forms suggested their uses for media record or medical uses among others [2,3] but lately, due to complementation with other lithographic techniques, it has been possible to achieve more complex and oriented patterns which generate a great expectative for their uses in interaction with magnetic and electronic circuits [4,5] or for tuning magnetic behaviors.

In our experiments we have been working with the block-copolymer polystyrene – poly 4 vinylpyridine (PS-P4VP) to obtain a large variety of structures by spin coating processes on Si substrates (see Figure 1). Thus, we have obtained micelles, horizontal or vertical cylinders, and complex nanorings, whose sizes and inter distances we are able to tailor in ranges of 30-110 nm of diameter by tuning their chemical properties (with the inclusion of different host molecules in the P4VP cores) and physical properties during spin coating. Furthermore, we have also studied the reproducibility of the different configurations in a variety of substrates with different chemical nature. Finally, we have also analyzed the possibility to obtain magnetic nanoparticles by incorporating magnetic salts with a chemical affinity for the P4VP domains.

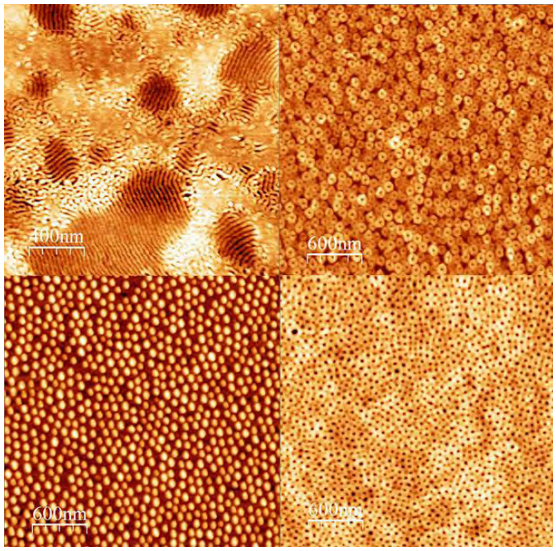

Fig 1. Atomic Force Microscope images of different structures obtained by PS-P4VP tuning (horizontal cylinders, nanorings, micelles and vertical cylinders).

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Growth and characterization of iron oxide nanoparticles embedded in silica sol-gel thin films

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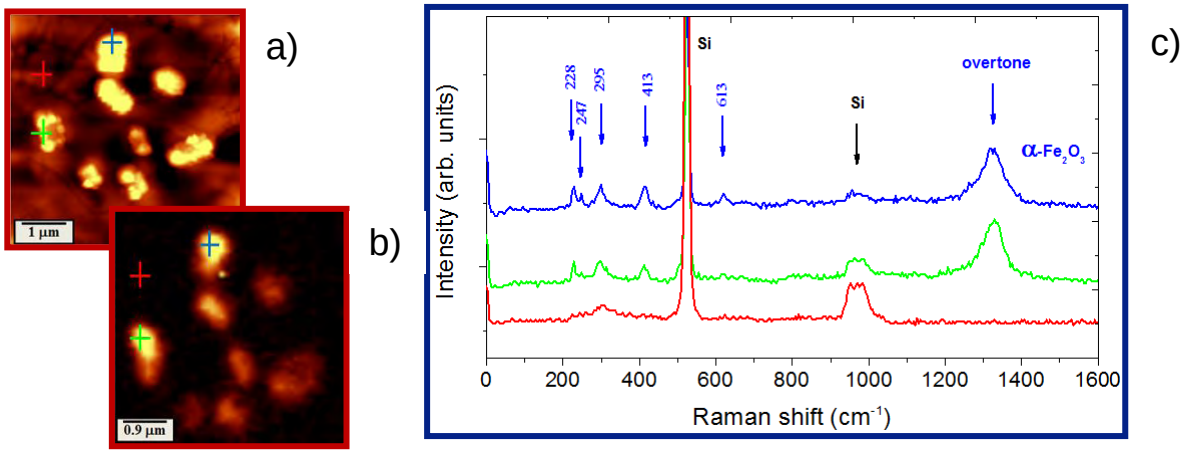

Fig.1. a) Imagen de topografía de AFM de nanopartículas de hematita que emergen de la matriz de SiO_2 sobre una oblea de Si(100) tratada a 1000ºC; b) Imagen Raman de la misma zona que la barrida con el AFM; c) Espectro Raman de las zonas marcadas en rojo (sílice), verde y azul (hematita)

Distintos polimorfos de Fe_2O_3 (α, β, γ y ε) muestran propiedades bioquímicas, magnéticas, catalíticas que los hacen muy aptos para determinadas aplicaciones técnicas y bioquímicas[1]. Existen diversos métodos relacionados con la síntesis de nanopartículas de óxido de hierro (III), y entre ellos destaca la técnica de sol-gel. Se trata de un método económico, con un amplio rango de variación de parámetros de síntesis y que nos permite trabajar a temperatura ambiente. Todos estos motivos lo convierten en un mecanismo adecuado para conseguir las diferentes fases de óxido de hierro (III). Además posee la ventaja, frente a otras técnicas, de que pueden obtenerse muestras en forma de polvo, en monolito o en película delgada, dependiendo de la aplicación. En este trabajo hemos conseguido sintetizar películas delgadas formadas por nanopartículas de todas las fases Fe_2O_3 embebidas en una matriz de sílice sobre Si(100). Hemos conseguido muestras monofásicas y en algunas ocasiones mezcla de varias, las cuales han sido caracterizadas por Difracción de Rayos X, Microscopía de Fuerzas Atómicas, Espectroscopía Mossbauer y Microscopía Confocal Raman. Todas ellas han sido técnicas esenciales para distinguir e identificar las diferentes fases del Fe_2O_3, que en algunos casos aparecen simultáneamente y dan lugar a una difícil caracterización del material.

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Photoemission electron microscopy study of magnetic domain structure in self assembled $La_{0.7}Sr_{0.3}MnO_3$ nano-islands

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The realization and characterization of mixed-valence lanthanum manganite based nanoscale features remains a challenge towards their implementation in real devices such as magnetic sensors, memories or magnetic tunnel junctions. In this work we present self-assembled ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) nanoislands (thickness ~10-40nm and lateral size ~50-200 nm) chemically grown using a very simple bottom-up methodology and we provide a comprehensive characterization of the system concerning its structural and magnetic properties [1].

Square-based (001) nanoislands (~80% of the total population) coexist with a minority (~20%) of triangle-based (111) nanoislands. These nanoislands appear strain-relaxed and exhibit the (001)LSMO[110]//(001)YSZ[100] and (111)LSMO[-112]||(001)YSZ[100] epitaxial relationship respectively, as measured through X-ray diffraction and TEM. SQUID magnetometry experiments have evidenced bulk-like magnetic performance of the nanoisland ensemble with Tc ~350 K. The chemical composition and the magnetic structure of individual LSMO nanoislands are explored using Photoemission Electron Microscopy (PEEM). X-ray absorption spectra (XAS) provide separate information of the surface and the bulk composition of the nanoislands and give evidence of Mn^{2+} present on the surface of otherwise stoichiometric nanostructures. Ferromagnetic domains less than 70 nm are resolved using X-ray magnetic circular dichroism (XMCD), which allows for the detection of magnetic vortex states in both $(001)_{LSMO}$ square and $(111)_{LSMO}$ triangular manganite nanoislands. The evolution of single nanostructures under in-plane magnetic field is seen to depend on the specific nanoisland size and geometry.

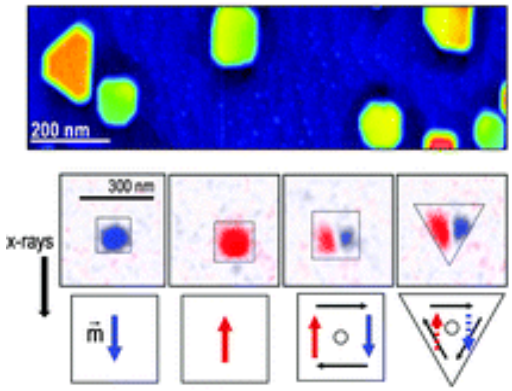

Figure 1. Magnetic domain structure of $La_{0.7}Sr_{0.3}MnO_3$ nanoislands extracted by XMCD measurements

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Uniaxial magnetic anisotropy in nanopatterned Co films

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We have investigated the formation, topography, composition and, magnetization reversal of nanoscale ripples on etched Co/Si(100) films. After growing these cobalt films, they were eroded *in situ* with Ar^+ beam (1.2keV, 0.1mA/cm^2) in grazing incidence with exposure times from a few minutes to an hour. The topographic characterization of those patterned surfaces was accomplished by atomic and magnetic microscopy resulting in a periodic array of quasi unidimensional and parallel Co wires running parallel to the ion beam direction. The amplitude and the periodicity of the ripples increase first with the etching time and for long irradiation times (~30 min) reach saturation values of about 10 nm and 80 nm, respectively. The angular dependent magnetization reversal behaviour was studied by vectorial-resolved Kerr magnetometry in the whole angular range. Very-well defined uniaxial magnetic anisotropy, with the magnetization easy axis (e.a.) along the wire, has been found for samples with a long erosion time (1 hour). The relevant mechanism during reversal changes from nucleation and further propagation of magnetic domains around the e.a. to rotation processes around the hard axis direction. Additionally, this angular dependence is also evidenced in magnetoresistance measurements. The results are discussed in the frame of a well-defined uniaxial magnetic anisotropy, arising from the quasi-linear array of nanowires, and ruling both magnetic and magnetotransport properties.

Tuning Topological Defects in Magnetic Stripe Domains of Lateral Multilayers with Perpendicular Magnetic Anisotropy

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Amorphous Nd-Co films with weak perpendicular magnetic anisotropy have been nanostructured with a periodic thickness modulation that results in the modulation of both stripe domain periods and in-plane magnetization component. The resulting system is the 2D equivalent of a strained superlattice with properties controlled by interfacial misfit strain within the magnetic stripe structure and shape anisotropy. Magnetic force microscopy measurements reveal that, depending on lateral multilayer period and in-plane applied field, it is actually possible to tune the magnetization reversal process and to control the nucleation of topological defects within the magnetic stripe domain pattern. In particular, for large enough periods, thin and thick regions switch independently during in-plane magnetization reversal and domain walls are created within the in-plane magnetization configuration coupled to variable angle grain boundaries and disclinations within the magnetic stripe domain patterns.

The process is mainly driven by the competition between rotatable anisotropy (that couples the magnetic stripe pattern to in-plane magnetization) and in-plane shape anisotropy induced by the periodic thickness modulation. However, as the structural period becomes comparable to magnetic stripe period, the nucleation of topological defects at the interfaces between thin and thick regions is hindered by a size effect and stripe domains in the different thickness regions become strongly coupled.

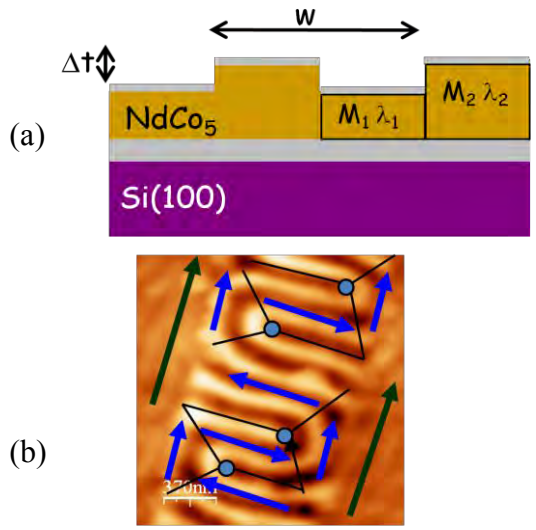

Fig 1. (a) Sketch of Lateral Magnetic Multilayer; (b) Topological defects in the stripe domain pattern of a NdCo lateral multilayer (1/2 disclinations coupled to 1/2 vortices).

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[2] A. Hierro-Rodriguez, G. Rodríguez-Rodríguez, J. M. Teixeira, G. N. Kakazei, J. B. Sousa, M. Vélez, J.I. Martín, L. M. Álvarez-Prado, and J. M. Alameda, J. Phys. D **46**, 345001 (2013)
[3] A. Hierro-Rodríguez, M. Vélez, R. Morales, N. Soriano, G. Rodríguez-Rodríguez, L. M. Álvarez-Prado, J. I. Martín, and J. M. Alameda, Physical Review B (en prensa)

Self-assembly of bicomponent supramolecular networks: adsorption height changes and their consequences

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Codeposition of two molecular species [CuPc (donor) and PFP (acceptor)] on noble metal (111) surfaces leads to the self-assembly of an ordered mixed layer with maximized donor-acceptor contact area. The main driving force behind this arrangement is assumed to be the intermolecular C-F··· H-C hydrogen-bond interactions [1]. Such interactions would be maximized for a coplanar molecular arrangement. However, precise measurement of molecule-substrate distances in the molecular mixture reveals significantly larger adsorption heights for PFP than for CuPc. Most surprisingly, instead of leveling to increase hydrogen bond interactions, the height difference is enhanced in mixed layers as compared to the heights found in single component CuPc and PFP layers, resulting in an overall reduced interaction with the underlying substrate. Such a change in the adsorption height of PFP is expected to affect interface phenomena. Our photoemission measurements show this effect is indeed measureable, as we find that the work function shift caused by deposition of PFP onto CuPc/Metal is smaller than what is found for the deposition of the same amount of PFP onto the bare metal substrate [2]. We hereby provide a direct measure of the effect of a molecule's adsorption height on vacuum level shifts and, in turn, interfacial energy level alignment.

[1] A. El-Sayed, P. Borghetti, E. Goiri, C. Rogero, L. Floreano, G. Lovat, D. J. Mowbray, J. L. Cabellos, Y. Wakayama, A. Rubio, J. E. Ortega, D. G. de Oteyza, ACS Nano **7**, (2013) 6914
[2] E. Goiri, M. Matena, A. El-Sayed, J. Lobo-Checa, P. Borghetti, C. Rogero, B. Detlefs, J. Duvernay, J. E. Ortega, D. G. de Oteyza, Submitted

Modificación de la hidrofilicidad de la superficie TiO2(110) mediante bombardeo iónico

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Existe una amplia literatura referente a la adsorción de agua en superficies de TiO_2(110) en presencia de una baja concentración de vacantes de oxígeno. Sin embargo, hasta el momento no existen trabajos que estudien la naturaleza de los procesos de mojado (*wetting*) sobre esta superficie en un gran rango de concentración de defectos bajo condiciones ambientales.

Recientemente nuestro grupo de investigación ha llevado a cabo estudios que concluyen que la superficie (110) del TiO_2, bajo grandes dosis de bombardeo iónico de baja energía (Ar^+), forma una capa pseudoepitaxial del subóxido TiO. En este trabajo se realiza el estudio de cómo estos cambios morfológicos y estructurales afectan a la hidrofilicidad de la superficie. Hemos llevado a cabo la caracterización estructural y química de la superficie mediante microscopía de fuerzas atómicas (AFM), espectroscopía Auger (AES) y difracción superficial de electrones lentos (LEED).

Se han realizado medidas a nivel macroscópico mediante un medidor de ángulo de contacto *Krüss DSA 100*, el cual nos permite medir el ángulo de contacto de gotas de unos pocos milímetros cúbicos de volumen. También se han realizado medidas a nivel microscópico observando la condensación de microgotas de vapor de agua sobre las superficies plana y bombardeada mediante microscopía óptica.

Los datos obtenidos muestran que la superficie modificada presenta un mayor ángulo de contacto, esto es, es más hidrofóbica. Esto es contrario a lo esperado si se tiene en cuenta que la literatura afirma que, en general, la introducción de defectos y la rugosidad producidas por medio de bombardeo iónico tienden a aumentar el grado de hidrofilicidad intrínseca de una superficie, pero no debemos olvidar que en este caso la modificación no ha sido sólo morfológica y/o química, sino también estructural.

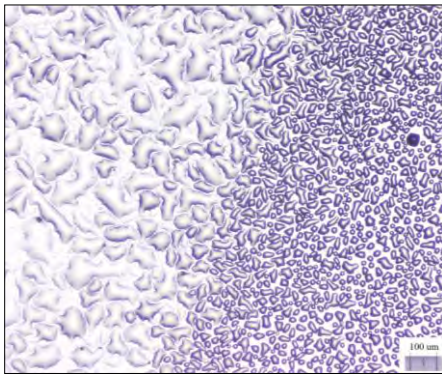

Fig 1. Imagen de microscopía óptica de microgotas de agua adsorbida sobre la frontera entre las superficies plana (izquierda) y bombardeada con iones de baja energía (derecha).

En cuanto a las imágenes de microscopía óptica, se observa que en los primeros pasos de condensación la cantidad de centros de nucleación de gotas es apreciablemente mayor en la superficie plana, mientras que conforme avanza la exposición las gotas en esta superficie tienden a coalescer más fácilmente, resultando finalmente en una menor densidad de gotas que en la superficie modificada, siendo también más extensas y de menor altura (ver Fig. 1).

Skin Layers in Multiferroic and Relaxor Single Crystals

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Skin effects are commonly observed in different types of single crystals: in regions close to the surface, structural and functional properties different from that of the bulk can be observed. In this presentation we want to overview the main features that characterize skin layers observed in different types of ferroelectric single crystals, from multiferroic materials such as $BiFeO_3$ to different examples of relaxors such as PZN-PT.

Skin layer of $BiFeO_3$ has been analyzed with different techniques from surface impedance and grazing incidence X-ray diffraction to atomic force based techniques such as Piezoresponse Force Microscopy (PFM). It has been demonstrated that the skin shows a specific phase transition at T* ~ 275 ºC below the bulk transition temperature, characteristic dielectric properties and a complex distribution of near-surface ferroelectric nanodomains that organize in a hierarchical metastructure on top of the existing bulk domains. [1], [2]

On the other hand, morphotropic phase boundary relaxors have been intensely studied for the last 15 years, on account of their giant electromechanical performance. The relaxation dynamics have traditionally been linked to the existence of both chemical and structural heterogeneity on a nanoscopic scale, with random bonds and random fields disrupting a true long-range ferroelectric ordering. For reasons that are as yet not understood, relaxor ferroelectrics display fairly thick surface layers ("skin layers") with different symmetry compared to bulk. [3] In this frame, PFM becomes a powerful tool to study the ferroelectric domain distribution and in general ferroelectric properties locally on the surface. In this presentation, I will introduce the technique of PFM and will show, in closer detail, the surface layer of these materials, and in particular the temperature dependence of its properties. Using a combination of temperature-dependent PFM and grazing incidence X-ray (XRD) we confirmed that the skin layer indeed has different symmetry and different domain structure as compared to the bulk, surviving to temperatures hundreds of degrees above the bulk, corroborating that skin layers have their own phase diagram quite independent from that of bulk.

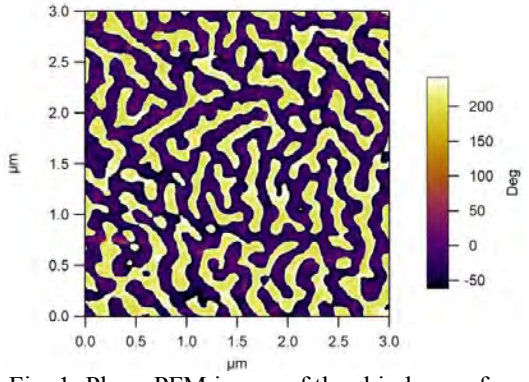

Fig. 1: Phase PFM image of the skin layer of PZN-PT measured at room temperature.

[1] X. Martí, *et al.,* Physical Review Letters **106** (2011), 236101.
[2] N. Domingo, *et al.*, Journal of Applied Physics **113** (2013) 187220.
[3] Xu, Guangyong, *et al.*, Applied Physics Letters **84**, (2004) 3975.

Thermoelectric properties of hole-doped $SrTiO_3$ thin films

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Two dimensional conductors are expected to show an improved thermoelectric performance due the positive effect of quantum confinement on the thermoelectric power, and the decrease of thermal conductivity by interface boundary scattering. The recent report of a large increase of the thermoelectric power in quantum wells of Nb-doped $SrTiO_3$ (STO), seems to be in agreement with this hypothesis [1]. However, extrinsic effects like the existence of oxygen vacancies that propagate away from the interface cannot be ruled out, and the results are far from clear.

Here we will present the thermoelectric properties (electrical conductivity, Seebeck coefficient, and Hall effect), of epitaxial thin-films of (La,Nb)-doped $SrTiO_3$ (STO). The films have been deposited by Pulsed Laser Deposition (PLD) on different substrates (STO, LAO...) in order to study the effect of tensile/compressive stress on the thermoelectric properties of the material. The oxygen pressure during the deposition was carefully controlled in order to tune the amount of oxygen vacancies and to compare with the cation doping. We have performed a systematic study of the transport properties as a function of thickness and doping, which along with the effect of stress, allows to understand the effect of charge density and dimensionality in an oxide system with promising thermoelectric properties.

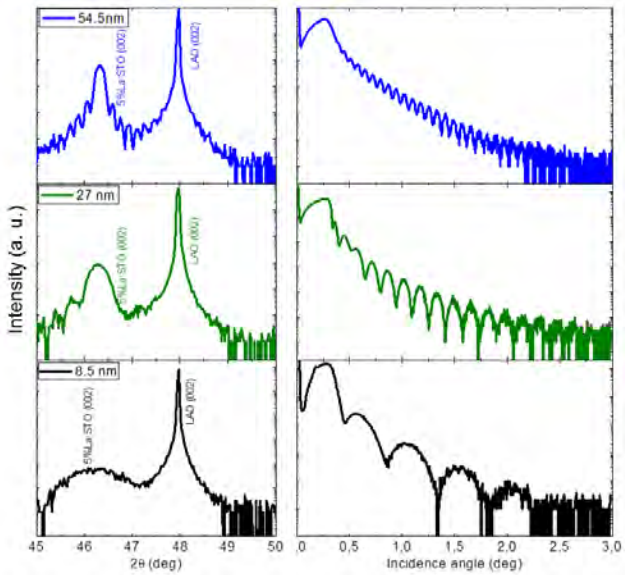

Figure. XRD and XRR of thin-films of La:STO with different thickness, deposited on LAO.

[1] H. Ohta et al. Nat. Mat. **6**, (2007) 129.

Controlling shot noise in double barrier epitaxial magnetic tunnel junctions

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We have recently shown that shot noise is an effective tool to study the statistics of electron tunnelling in single and double barrier magnetic tunnel junctions [1-2]. This talk discusses our recent results on the magnetic control over shot noise in epitaxial double barrier magnetic tunnel junctions [3-4]. We demonstrate that shot noise in Fe/MgO/Fe/MgO/Fe double barrier magnetic tunnel junctions is determined by the asymmetry between both tunnel barriers, the relative magnetic configuration and is influenced by quantum well states in the central layer. The proposed theoretical model of sequential tunnelling through the system, with spin relaxation taken into account, successfully accounts for the experimental observations for all four different magnetic states in the applied bias range, for which the influence of tunnelling through barrier defects and resonant states inside the central electrode is negligible. These results open up a new perspective to engineer fundamental, out of equilibrium, noise mechanisms utilizing hybrid spintronic structures.

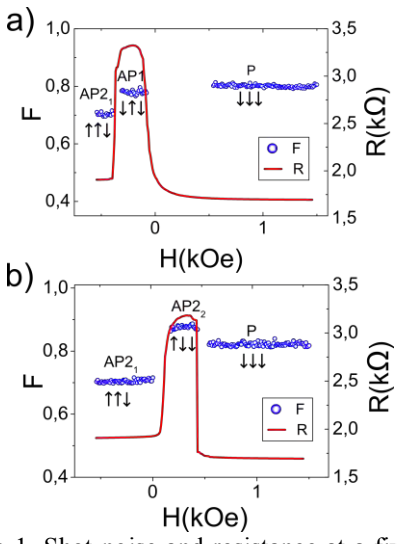

Fig 1. Shot noise and resistance at a fixed current during a magnetic field sweep at T=0.3K (a) from positive to negative values and (b) from the $AP2_1$ at negative fields back to positive fields.

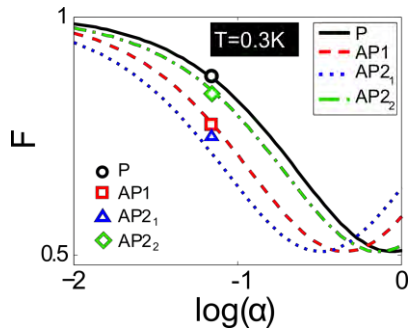

Fig 2. Comparison of the experimental values (points) and the theoretical results (lines) for the Fano factors measured in a double barrier magnetic tunnel junction at T=0.3K. An estimate of the asymmetry between the barriers and the spin relaxation time is obtained from the fit.

[1] R. Guerrero, et al., Phys. Rev. Lett. **97**, 0266602 (2006).
[2] R. Guerrero, et al., Appl. Phys. Lett. **91**, 132504 (2007).
[3] J.P. Cascales, et al., Phys. Rev. Lett., **109**, 066601 (2012).
[4] J.P. Cascales, et al., IEEE Trans. on Magnetics, **49**, 4347 (2013)

Use of lithium fluoride in organic spintronics

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Polar layers are currently used in organic electronics to improve charge injection from metal electrodes into organic semiconductors (OS). These layers can be produced by inserting LiF, Mg, Cs, etc in the interface metal/OS. In particular, the effect of LiF on Alq3 -tris(8-hydroxyquinolinato)aluminium- based devices with aluminium electrodes has been broadly studied. LiF produces a shifting of the vacuum level of the OS which lowers the barrier height for electron injection.[1]

The use of LiF has also been extended to organic spintronics.[2] However, the effect of LiF on ferromagnetic electrodes has not already been well characterized. We use different techniques including X-ray absorption measurements and spin-polarized neutron reflectometry to fill this gap. We find that some chemical reactions can take place depending on the order of deposition of the materials. It allow us to explain the unique magnetotransport properties of LiF-treated organic spin valves and magnetic tunnel junctions.

[1] D. Yoshimura et al. Synthetic Metals 102, 1145 (1999).
[2] Schulz et al. Nat. Mater. 10, 39 (2011)

New experimental set-up to measure thermoelectric properties of films under sulphur atmosphere at moderate temperatures.

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Metal-based chalcogenides are usually considered to be used in thermoelectric applications due to their adequate transport properties. However, it is needed to find less expensive and non toxic chalcogenides with better transport properties to achieve a major implementation at different applications. To this aim, research is focused on sulphide compounds due to the abundance, low toxicity and cheapness of sulphur. Sulphides are frequently formed by a solid-gas reaction controlled by the sulphur pressure ($P(S_2)$) and metal temperature (T) that define the formed phase and subsequently, the thermoelectric properties. Therefore, an "in situ" measurement system of the transport properties during the sulphuration process is required to investigate, in accurately way, the thermoelectric properties of the sulphide phases formed at different $P(S_2)$ and T as well as the formation mechanism.

However, "in situ" thermoelectric properties measurements are performed under an inert gas (He, N_2) or vacuum but not under gases like sulphur due to its very high reactivity, complicated pressure control, etc. In this work, we present a novel experimental system able to monitor the transport properties of metallic thin films under a sulphur atmosphere. Resistance and thermopower could be measured up to 400 ºC and $P(S_2) < 10$ mb. Film temperature and sulphur pressure are controlled in an independent way. Experimental set-up was calibrated by measuring the transport properties of palladium and several semiconductor films ("n" and "p" type) under different atmospheres (He and air), pressures and temperatures. "In situ" transport properties measurements obtained during sulphuration of palladium films will be shown and compared to previous results. Results provide useful information about the metal sulphuration process (phases formed and their thermoelectric properties).

Acknowledgements

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Spin Hall magnetoresistance as a probe for surface magnetization

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During the last decade, there has been an extensive study on how to create and detect pure spin currents, being the spin Hall effect (SHE) and inverse spin Hall effect (ISHE) in non-magnetic (NM) metals with high spin-orbit coupling a promising approach [1]. Recently, a new magnetoresistance effect in NM/ferromagnetic insulator (FMI) bilayers has been discovered: the spin Hall magnetoresistance (SMR) [2,3]. The SMR arises from the simultaneous effect of SHE and ISHE in the NM in combination with the interaction of the generated spin current with the FMI. Depending on the magnetization orientation of the FMI, this spin current will be absorbed or reflected at the NM/FMI interface yielding a change in the resistance (Fig. 1).

In this work, we address this issue by measuring the angular dependence of the magnetoresistance of thin Pt stripes deposited on (001) and (111) epitaxial $CoFe_2O_4$ (CFO) films. Results are well described by the SMR model, allowing us to extract the spin mixing conductance (Gr), which accounts for the contribution of the NM/FMI interface. We find Gr to depend on the crystallographic orientation of the FMI, being $Gr < 6.07 \cdot 10^{13}\ \Omega^{-1}m^{-2}$ for (111) and $Gr < 1.5 \cdot 10^{15}\ \Omega^{-1}m^{-2}$ for (100) [4].

Additionally, the magnetic properties of CFO films are compared to the magnetoresistance of CFO/Pt bilayers. Data shows that field-dependent SMR, although reminiscent of the bulk magnetization process, contains distinctive features. We claim that they reflect the surface magnetization of CFO films, which, as typical of spinel ferrites, largely differs from bulk [4]. Therefore, SMR can be used as a probe for complex surface magnetization that cannot be detected with standard magnetometric techniques.

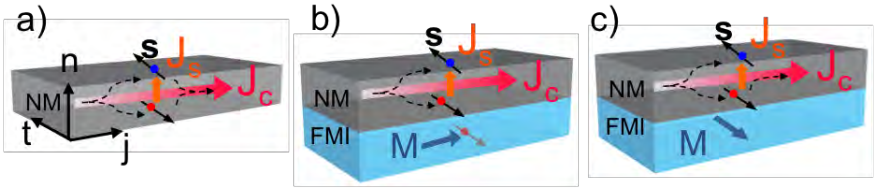

Fig 1. Schematic representation of the SMR. (a) A spin current j_s is created in a NM material with strong spin orbit coupling. The spin current is reflected back at the surfaces creating an additional charge current. (b) The spin current is absorbed if the magnetization of the FMI is perpendicular to the spin polarization. (c) The spin current is reflected if the magnetization of the FMI is parallel to the spin polarization.

[1] T. Kimura et al., Phys. Rev. Lett. **98**, (2007) 156601.
[2] H. Nakayama et al., Phys. Rev. Lett. **110**, (2013) 206601.
[3] N. Vlietstra et al., Phys. Rev. B **87**, (2013) 184421.
[4] M. Isasa et al., arXiv:1307.1267.

Energy-harvesting at the nanoscale

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Energy harvesting is the process by which energy is taken from the environment and transformed to provide power for electronics. Specifically, the conversion of thermal energy into electrical power, or thermoelectrics, can play a crucial role in future developments of alternative sources of energy. Unfortunately, present thermoelectrics have low efficiency. Therefore, an important task in condensed matter physics is to find new ways to harvest ambient thermal energy, particularly at the smallest length scales where electronics operate. To achieve this goal, there is on one hand the miniaturizing of electrical devices, and on the other, the maximization of either efficiency or power the devices produce.

We will present the theory of nano heat engines able to efficiently convert heat into electrical power. We propose a resonant tunneling quantum dot engine that can be operated either in the Carnot efficient mode, or maximal power mode. The ability to scale the power by putting many such engines in a "Swiss cheese sandwich" geometry gives a paradigmatic system for harvesting thermal energy at the nanoscale, see Fig. 1.

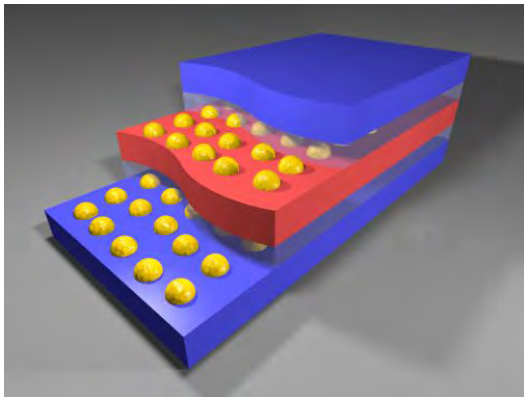

Fig 1. Sketch of a "Swiss cheese sandwich" energy harvester. Electron flow is generated between cold reservoirs (blue layers) which are connected via self-assembled quantum dots (yellow) embedded in an insulating matrix (transparent) to a central hot cavity (red).

Alternative configurations based on resonant tunneling through quantum wells provide a comparable thermoelectric performance with the advantage of being easier to construct.

[1] A. N. Jordan, B. Sothman, R. Sánchez, M. Büttiker, Phys. Rev. B 87 (2013) 075312.
[2] B. Sothman, R. Sánchez, A. N. Jordan, M. Büttiker, New J. Phys. 15 (2013) 095021.

Crystal structure and magnetic frustration in Co-ferrite nanoparticles

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Ferrite nanoparticles (NPs) with composition MFe_2O_4 (M= Fe, Co) are currently attractive nanomaterials due to their potential applications such as the detection of biomolecules by magnetic separation, improving the contrast in nuclear magnetic resonance imaging and magnetic hyperthermia **[1].** In particular, Co-ferrite NPs are suitable for those applications because of their high values of the magnetocristalline anisotropy, saturation magnetization and the magneto-optical coefficients **[2]**. Moreover, Co-ferrite NPs show a high magnetic response even for a few nanometers in size.

However, the studies previously published on those systems show a great variety of results for the magnetic properties suggesting that the synthesis of those materials is strongly affected by factors limiting the reproducibility. We have addressed this issue by studying three samples of Co-ferrite NPs prepared by high-temperature decomposition method in an organic solvent with different reactants aiming at comparing the role of the organic precursors on the final magnetic and structural properties **[3]**. The S1 sample was synthesized by a conventional method, S2 was prepared from the decomposition of Co and Fe oleates, and the S3 one from Co and Fe acetylacetonates. Oleic acid was used as a surfactant in all three cases. Structural characterization (HRTEM, DRX, EELS) for S2 and S3 samples shows poor crystal quality, indicating the presence of several crystallographic defects and/or domain boundaries throughout the whole NPs and excluding the formation of core-shell structures. In contrast, S1 NPs are single crystals almost free of crystallographic defects. Interestingly, while S1 shows magnetic properties close to those of the bulk counterpart, S2 and S3 display marked particle-like features suggesting a strong relationship between crystal structure and magnetic response. For instance, S3 sample exhibits spin glass-like behaviour at low temperature associated with a highly defective crystallographic structure which is responsible of the formation of a spin-glass-like state through the competition among ferrimagnetically ordered domains. The key role of the crystal quality is thus suggested, because particle-like behaviour above about 5 nm in size is observed only when NPs are structurally defective. This is crucial to prepare NPs with enhanced magnetic properties and suitable for biomedical and technological applications.

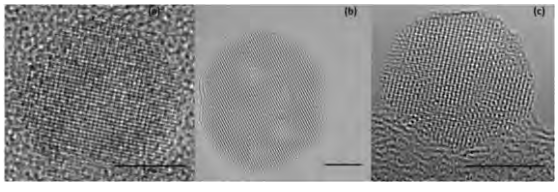

Figure 1.TEM images of Co-ferrite nanoparticles. (a) S1, (b) S2 (c) S3

[1] C. Sun et al., Advanced Drug Delivery Reviews 60 (2008) 1252-1265
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[3] N.Pérez et al., Phys. Chem. Chem. Phys., 13 (2011) 19485-1948.

Antiferromagnetic spintronics

I. Fina[1,*], X. Marti[2,3,4], D. Yi[2], C. Rayan-Serrao[2], J. Liu[2], Jiun-Haw Chu[2], S.J. Suresha[2], J. Zelezny[4], T. Jungwirth[4,5], J. Fontcuberta[2], R. Ramesh[2]

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Magnetic semiconductors entwine two of the most successful concepts in both fundamental physics and industrial applications where ferromagnetic materials have played an undismissable role. Recently antiferromagnets have been proposed as alternative material systems [1,2]. Antiferromagnetic spintronics have been demonstrated by the fabrication of tunnel devices [3,4], atomic-size proof-of concepts [5], even devices without auxiliary ferromagnetic layers [6]. Here we survey the progress in antiferromagnetic spintronics and we present the control of the electrical conductivity of an antiferromagnetic semiconductor by manipulating the magnetic state of a contiguous ferromagnetic layer acting as a spin-based gate.

We present an oxide-based fully epitaxial heterostructure, its structural characterization and the electrical measurements showing a direct link between state of the ferromagnetic gate and ohmic resistance of the semiconductor, even displaying distinct remnant resistance states. We will also show that distinct remnant states can also been obtained at room temperature without requirement of the spin-gating element, promising potential applicability.

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Spin waves along topological domain walls

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The microwave dynamics of the single magnetic vortex has been actively investigated as a new basic element of spin torque oscillators and novel magnetic memories [1-3]. Recent reports show that thin circular dots may also accommodate two magnetic vortices as a metastable state [4]. We present an investigation of the magnetization dynamics in circular Permalloy (Py) dots in the single vortex (SV) or double magnetic vortex (DV) states by means of broadband ferromagnetic resonance and micromagnetic simulations. In the metastable DV configuration in circular dots we have observed a new type of quasi 1D spin waves excited along the domain walls (Fig.1a) connecting the vortices and edge half-antivortices [5].

We have also investigated broadband magnetization response of equilateral triangular 1000 nm Py under an in-plane magnetic field, applied parallel (buckle state) and perpendicular (Y state) to the triangles base. Micromagnetic simulations identify edge spin waves (E-SWs) in the buckle state as SWs propagating along the two adjacent edges. These quasi one-dimensional spin waves emitted by the vertex magnetic charges gradually transform from propagating to standing due to. Spin waves in the Y state have a two dimensional character. Our findings provide insight into dynamics of magnetic elements with topologically pinned domain walls.

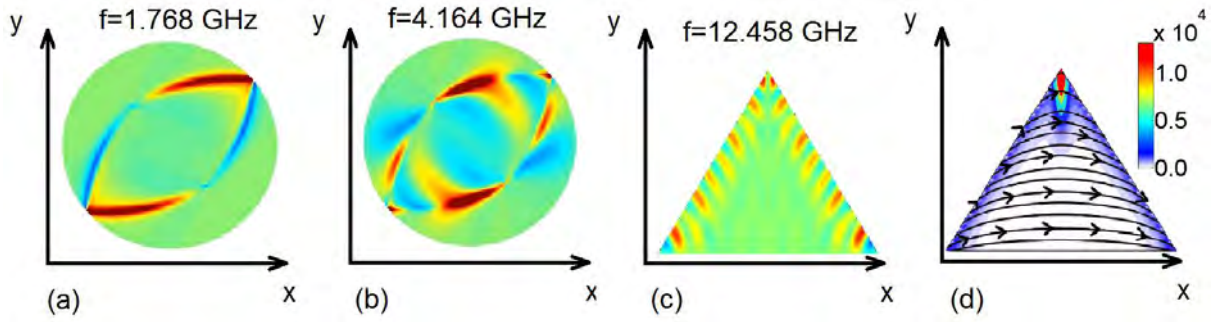

Fig1. (a) and (b) Spin waves (Winter magnons), dynamic magnetization component in x direction in a double vortex state circular dot for two eigenfrequencies, (c) Buckle state in a triangular dot, (d) Exchange energy density (colors, in J/m^3) and magnetization (arrows).

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Influence of composition and geometry on magnetic properties of ordered NiCu nanowires arrays

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In the last years, studies on ferromagnetic-nonmagnetic multilayer and binary nanowires arrays, including CoCu, FeAg, CoAg, CoPd and NiCu [1-4], have been reported in the literature due to their interesting magnetic and magnetotransport properties. From the large variety of magnetic systems, NiCu alloy is characterized by high strength, corrosion resistance, good wear resistance, giant magnetoresistance and good magnetic properties [5].

In the present work, arrays of $Ni_{100-x}Cu_x$ nanowires with various diameters, lengths and different composition have been fabricated by co-depositing Ni and Cu into porous anodic alumina membranes (AAO) in order to determine their magnetic behavior.

The composition of the nanowires (0>x>75) was controlled using different electrolytes, the lengths (0.15-28 μm) with the time of electroplating and the diameters (35-80 nm) using membranes with different pores sizes (Figure 1).

The magnetic measurements show that the increase of Cu content into the alloy up to 50% improves the magnetic properties of NiCu nanowires, such as coercivity and squareness (Mr/Ms), along the axis. For x>50, these properties decrease and the easy axis become oriented perpendicular to the wires.

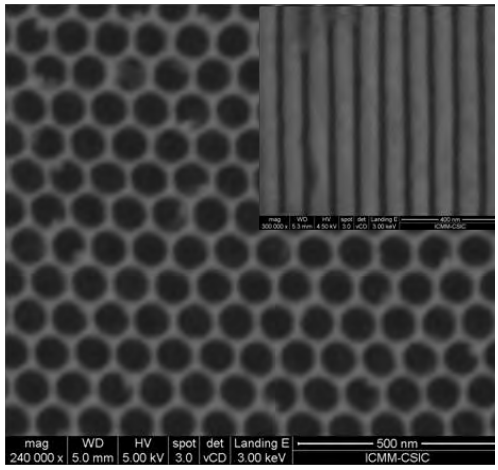

Fig 1. SEM image of the top view of an AAO membrane and the cross section of NiCu nanowires.

Magnetic properties of NiCu alloy nanowires can be tailor further by tuning the geometrical parameters of nanowires such as lengths and diameters. The coercivity and remanence increase by reducing the length (L<1μm) and also by decreasing the diameter. The results are interpreted considering the crystal structure (magnetocrystalline anisotropy) and geometry of nanowires (shape anisotropy).

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Large room-temperature electroresistance in $BaTiO_3$ tunnel junctions

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In the past few years, ferroelectric tunnel junctions (FeTJs) have attracted considerable interest for potential application in nanoelectronics and data storage. The electrical modulation of conductivity in FeTJs in response to a ferroelectric polarization of the tunneling barrier, phenomenon known as the tunneling electroresistance (TER) effect, is being considered for binary data storage and as a memristor for neuronal network emulation. Although TER values as large as 7.5 10^4 % have been reported using conductive nanometric tips as top electrodes, TER is found to be rapidly suppressed when contacts of the range of 0.1 μm^2 are used in real capacitor-like geometry, thus challenging progress on practical implementation of FeTJs.

Here we report on the fabrication and the room-temperature tunneling characteristics of $Pt/BaTiO_3/La_{0.7}Sr_{0.3}MnO_3//SrTiO_3(001)$ FTJs (junction areas from 4 to 1600 μm^2), grown by combined use of pulsed laser deposition and sputtering techniques with different thicknesses of the $BaTiO_3$ ferroelectric tunneling barrier. PFM measurements confirm a robust polarization. *I-V* curves have been recorded after applying a poling voltage, which reverses the barrier polarization. Clear TER effect has been observed at room temperature for all investigated samples (2, 3 and 4 nm thick BTO barrier). *I-V* characteristics recorded both in on and off resistance states, show typical features of tunnel behavior, indicating that in our large-area devices, tunneling dominates room-temperature transport. Resistance vs. poling voltage loops unambiguously show that the two resistance states correspond to the two ferroelectric polarization states of the ferroelectric $BaTiO_3$ barrier. Moreover, we observed an exponential increase of TER with the barrier thickness, in agreement with theoretical predictions. We obtained extremely large room-temperature TER values, (up to 10^4%) in micro-devices paves the way to the consideration of such a kind of ferroelectric devices for storage applications.

Injection, transport and manipulation of pure spin currents using Lateral Spin Valves

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Creation and manipulation of pure spin currents is a key ingredient in spintronics. A way to create such spin currents is by electrical spin injection and detection using ferromagnetic (FM) / non-magnetic (NM) lateral spin valves (LSVs) in a non-local geometry [1]. In this work, LSV devices are fabricated by using a two-step electron-beam lithography process. In the first step, FM electrodes, such as cobalt (Co) or permalloy (Py), are deposited and, in the second one, a NM metal, such as copper (Cu) or aluminum (Al), is put on top. In these devices, the spin signal is measured at different distances, from which the current spin polarization of the FM (α_{FM}) and the spin diffusion length of the NM (λ_{NM}) are obtained.

The analysis of Py/Cu and Co/Cu LSVs allows us to study and compare the spin injection properties of both FM materials [2]. α_{Py} and α_{Co} are reported for the first time as a function of temperature (T). In the case of Py, the comparison of α_{Py} and its conductivity agrees well with the prediction given by the standard two-channel model [3], allowing the detection of an underestimation of α_{Py}.

By systematically changing the dimensions of the Cu channel, the spin transport in Cu is also studied [4], attributing the T-dependent spin relaxation to phonons, and the T-independent one to defects, which are dominated by grain boundaries. In addition, we find that the spin transport mechanisms of Cu are not affected by the used FM material [2], identifying the intrinsic magnetic impurities present in Cu as the responsible for an anomalous maximum of λ_{Cu} at low T.

Finally, several ways for manipulating pure spin currents are explored, such as the application of an out-of-plane magnetic field (Hanle effect) or the use of a ferromagnetic insulating substrate. This will open ways to novel applications.

Supported by EU Marie Curie actions, Basque Government, Spanish MICINN.

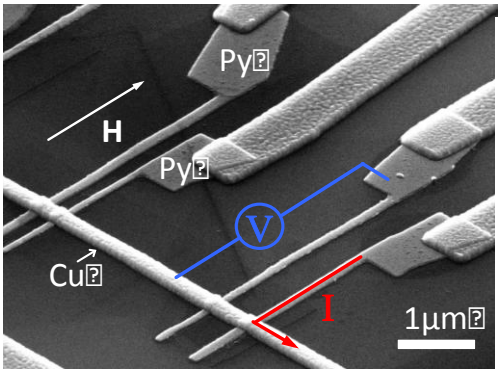

Fig. 1. Scanning electron microscope image of a sample showing two lateral spin valves. The nonlocal measurement configuration, materials, and the direction of the applied magnetic field H are shown.

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Giant temperature sensitivity of the Spin Reversal Field in epitaxial Chromia films

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The antiferromagnetic (AFM) insulator a-Cr_2O_3 (chromia) is an archetypical magnetoelectric (ME) material. Recently, strong interest in ME antiferromagnets revived, which was fueled by their potential for ultra-low power dissipation spintronic devices.[1, 2] However, these materials are also very interesting due to their fundamentally unique properties. In particular, the peculiar symmetry of ME antiferromagnets gives rise to a spin-polarized surface or boundary magnetization (BM) if the antiferromagnet is in one of its two degenerate single domains states, a fact that was only recently experimentally verified.[3,4,5] In this work we demonstrate that in the case of chromia (0001) thin films, which we have grown by means of sputter deposition and high temperature annealing, a moderate magnetic field can suffice to select and switch between opposite AFM single domain states due to their corresponding BM. This magnetic field-induced reversal of the surface spin polarization is studied as a function of temperature via magnetometry for chromia films of various thicknesses. In our experiments, we demonstrate that a reversal solely by magnetic fields can be achieved in sufficiently thin films, which is distinctively different from this materials' bulk behaviour where switching between time-reversed single domain states requires the simultaneous presence of electric and magnetic fields. In our detailed experiments, we furthermore observe a giant sensitivity of the coercive field on temperature, as can be seen in figure 1. This extremely large effect is an at least ten-fold increase over the temperature dependent change in coercivity measured for materials that are currently investigated as media for energy assisted magnetic recording. Thus, magneto-electric antiferromagnetic thin films could also be considered as promising candidates for energy assisted magnetic recording media.[6]

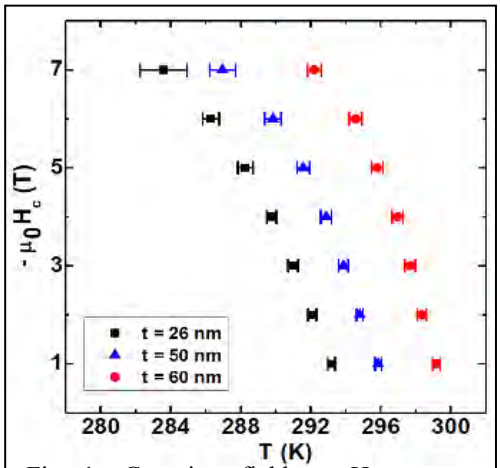

Fig 1. Coercive field, $-\mu_0 H_C$, versus temperature T for different film thickness

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Sulfuros metálicos como materiales termoeléctricos: Trisulfuro de Titanio (TiS_3)

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Los fenómenos termoeléctricos y sus aplicaciones, aunque conocidos desde el siglo XIX[1], no han sido considerados seriamente como posible fuente de energía hasta ahora. Sin embargo, recientemente se está impulsando la investigación en materiales termoeléctricos debido a la actual crisis energética y a la necesidad de aprovechar todas las fuentes posibles de energía. Los requisitos que debe cumplir un material para ser considerado adecuado para la obtención de energía eléctrica en dispositivos termoeléctricos son, básicamente: alto coeficiente Seebeck (S) y baja resistividad eléctrica (ρ) y térmica (κ). Estos parámetros definen el factor de potencia ($S^2\rho$) y la figura de mérito termoeléctrica ($ZT = \frac{S^2\rho}{\kappa}T$).

En este trabajo presentamos el TiS_3 como material termoeléctrico. Este material ha sido preparado en volumen, en película delgada y en forma de fibras (micro y nano fibras), a partir de la sulfuración de polvo, película delgada y lámina de Ti, respectivamente. El material se ha caracterizado estructuralmente mediante difracción de rayos X, comprobándose la existencia una sola fase: TiS_3 monoclínico. Se han medido sus propiedades eléctricas y su coeficiente Seebeck. Se ha comprobado que es un semiconductor tipo n con un coeficiente Seebeck a temperatura ambiente en torno a 0.7mV/K en volumen que aumenta hasta casi 1mV/K en forma de microfibras.

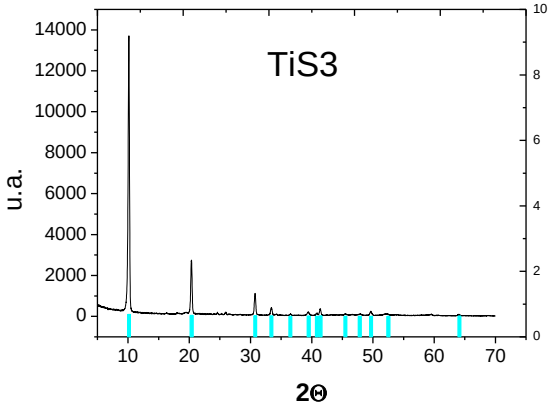

Fig.1 Patrón de difracción de rayos X de polvo de TiS_3.

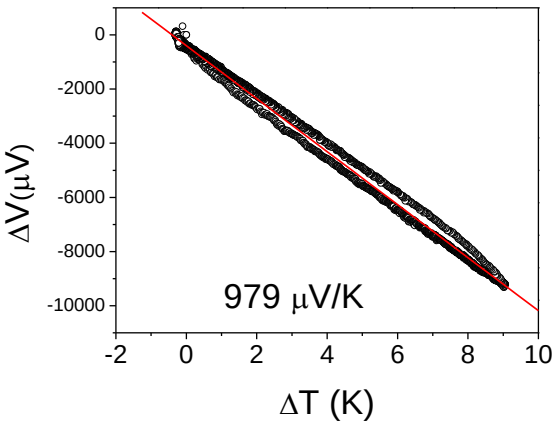

Fig.2. Medida del coeficiente Seebeck de fibras de TiS_3.

En la comunicación se presentarán y compararán las propiedades de este material en las tres formas en las que se ha obtenido.

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Magnetization reversal through multivortex states in circular Co dots with nanoholes

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Control over the magnetic state and reversal process of magnetic nanostructures is becoming an increasingly important aspect for new magnetic and spintronic devices. The ability to capture magnetic vortex cores in circular dots with artificial defects (holes) has been demonstrated in different configurations for a single vortex state [1,2].

We investigate the influence of artificial pinning centers in multi vortex states present in the magnetization reversal process of circular Co dots. Dots with centrally symmetric single, double or triple artificial pinning centers have been prepared using focused ion beam milling and investigated via in-plane magnetoresistance and broadband susceptibility measurements. We have found that Co dots with two and three nanoholes inclined at 45º with respect to the external magnetic field show reproducible step-like changes in anisotropic magnetoresistance (AMR) and magnetic permeability due to abrupt transitions through different intermediate magnetization configurations. Numerical calculations of AMR using micromagnetic simulations allow for visualizing the magnetization state at intermediate multivortex states.

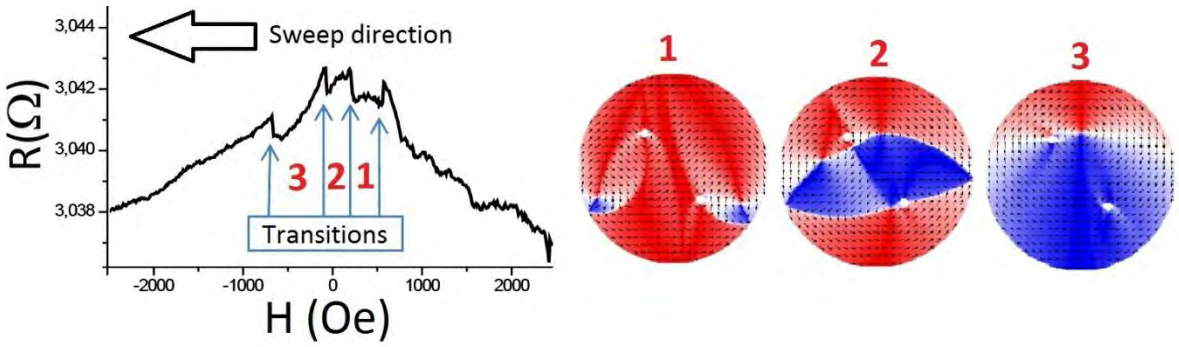

Fig 1. Measured AMR curve for a dot with two holes at 45º respect to applied field. Four abrupt transitions can be seen. The numbers between the transitions correspond to the simulated magnetic states, corresponding to: 1, a double vortex state. 2, three vortices. 3, a single vortex shifted from the center.

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Uniaxial Strain Control of Metal Insulator Transitions in Sr_2IrO_4 thin films

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Recent studies suggest that manipulation of the epitaxial strain can tune the electronic structure of the Jeff = ½ Mott insulator Sr_2IrO_4, which is a transition metal oxide that exhibits an exotic insulating state [1,2]. When thin films are grown on a substrate the mismatch between the lattice constant of the substrate and lattice constant of the thin film material induces an in-plane strain in order to achieve epitaxial growing. The in-plane lattice mismatch between Sr_2IrO_4 and the substrates can exert tensile or compressive strains to the film. On the other hand, mechanical stimuli induced by the tip of an atomic force microscopy (AFM) is the basis for the generation of different types of phenomenologies, from flexoelectric fields that can lead to mechanical writing in ferroelectric materials [3] to piezochemical effects due to the dynamics in ionic systems [4].

In this work, we present a novel technique to induce an insulator-to-metal transition by applying uniaxial pressure to the material through an Atomic Force Microscope (AFM) tip. We achieve the reversible mechanical control of dielectric gap in a semiconductor oxide that lead to metal-insulator transitions induced by uniaxial stress, demonstrating that local electronic structures can be locally changed by applying uniaxial pressure through an AFM tip. The AFM tip also acts as a sensor and transport measurements through the AFM tip are done through different approaches. In all cases the experimental setup consist of the sample and tip placed in series resulting in a capacitor where the tip is the top electrode and an LSMO thin film substrate between SIO and STO is the bottom electrode. While the features of the I(V) for the lowest applied forces resemble those of a semiconductor, linear Ohmic behavior is achieved for increasing forces with increasing slopes. From the obtained results, we observed a significant and reversible decrease of the resistance of the Sr_2IrO_4 thin film as a function of increasing mechanical loading force on the AFM tip. We attribute this behaviour to an insulator-to-metal transition caused by pressure induced changes in the Ir-O-Ir bond angle in the plane which produce a closure of the band gap.

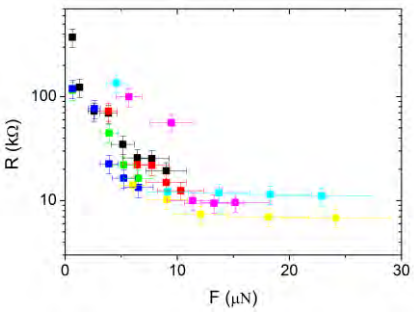

Fig 1. Resistance as a function of the applied force through an AFM onto Sr_2IrO_4 thin film.

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[5] L.L.M acknowledges financial support from the MINECO under project MAT2012-33207.

Microstructure and analysis of aluminum-silicon interface on polished and textured CZ silicon by screen-printing and dispensing technology

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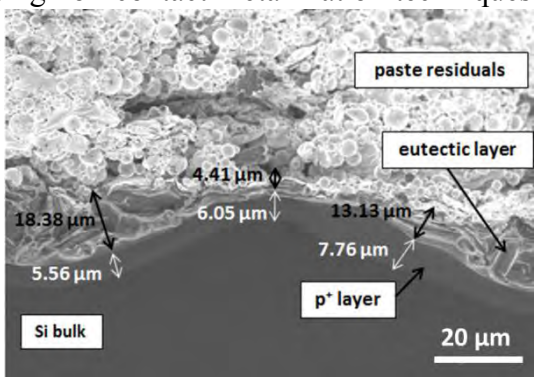
The Al-Si phase diagram system is a simple binary eutectic with limited solubility of aluminum in silicon and limited solubility of silicon in aluminum. The alloying process of screen-printed aluminum on silicon wafers during a short firing step of some seconds in a conveyor belt furnace has been used for many years in industrial solar cell standard production lines to form the p^+-doped BSF (Back Surface Field). This alloying process has been explained in detail using the Al-Si binary phase diagram. The analysis of this aluminum alloying has been studied by many authors using the screen-printing technology [1] with the aim to serve as metallization of the wafers or formation of front and back surface fields. On the other hand, dispensing technology offers an alternative to screen-printing technology without mesh marks and paste spreading, although pastes used in this technology must be adapted from screen-printing ones by modifying the rheology. For forming local metal contacts and so on the LBSF (Local Back Surface Field), the dielectric layer usually has to be locally removed before the aluminum screen-printing e.g. by etching paste or laser technique. Process parameters involved by these techniques seem to influence the local contact formation substantially. Because of that, in this work the local contacts formation was carried out by fire through contact method. Thin silicon wafers are a way to reduce costs in the raw material, but the bowing of such wafers after metallization causes its breaking in most of the cases and also microbreaks in the structure affecting to the lifetimes and to the efficiency of the final solar cell. This effect can be reduced by using non-contact metallization techniques like dispensing technology [2, 3].

We present a study of the microstructural interface between aluminium and silicon formed after screen-printing and also drop-on-demand technology (DOD), which is a dispensing technology, following by firing of Al pastes on polished and textured silicon. The same aluminium paste was studied with the aim to serve for both processes without any modification. Finally we tested the aluminium paste as fire through contact paste using silicon rich oxy-nitride (SiriON) as passivation layer.



SEM picture of an FTC cross-section

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Temperature dependence of the spin Hall angle in Pt and Au

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The discovery of the spin Hall effect (SHE) has introduced a novel way to generate and detect pure spin currents, which are key elements in the field of spintronics. When a charge current flows through a material with a strong spin-orbit interaction, a transverse spin current is created via the direct SHE (DSHE). The reciprocal effect, in which a charge current is created from the flow of a pure spin current, is known as the inverse SHE (ISHE). The main advantage of exploiting the SHE is that the use of ferromagnetic (FM) elements and external applied magnetic fields could be avoided [1].

In this work, we have studied the SHE in two transition metals (TM) using a device based on a lateral spin valve (LSV) geometry (Fig. 1). The LSV consists of a FM electrode (permalloy) which is used as a spin-polarized current injector, a NM channel (copper) which transfers the accumulated spins and a detector which is a TM electrode with high spin-orbit coupling. One of the studied metals is platinum (Pt), which is one of the most studied materials showing SHE, although there is a huge controversy regarding its magnitude [2]. The other metal is gold (Au), which is interesting because, even with a strong spin-orbit coupling, it shows a relatively large spin diffusion length. The spin Hall angle, which gives the efficiency to convert charge current into spin current, has been obtained as a function of temperature for both materials, being the first time that it is reported for the case of Au.

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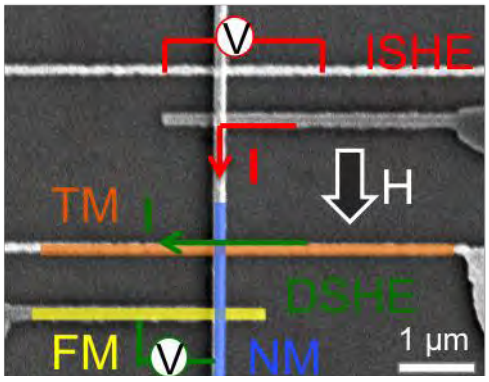

Fig. 1. Scanning electron microcope image of a sample with two devices to measure the SHE. The top device shows the schematic representation for detecting the ISHE, while the bottom device shows the DSHE detection scheme.

High-vacuum annealing reduction of Co/CoO Nanoparticles

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Co/CoO magnetic nanoparticles have been cluster-assembled by beam deposition forming porous films, which were subsequently subjected to thermal treatments in high-vacuum. X-ray diffraction (XRD), transmission electron microscopy (TEM), electric transport and magnetic measurements (with a focus on the exchange-bias phenomenon) have shown that for high-vacuum annealings at temperatures equal or higher than 360 ºC the CoO phase is mostly reduced to metallic Co without requiring the presence of an external reducing agent. Additionally, there was a certain degree of particle coalescence, resulting in the formation of larger and more crystalline nanoparticles with increasing annealing temperature, also more evident for temperatures ≥ 360º C. The combination of these chemical, morphological and crystallographic changes yields drastic variations in the exchange-bias field and saturation magnetization (which are, therefore, demonstrated to be sensitive probes for the studied reduction/oxidation processes), as well as in the electrical conductivity and in the stability of the sample against subsequent re-oxidation in air. Figure 1 displays a graphic summary of these changes, with the magnetic hysteresis loops, XRD patterns and TEM images for one of the studied samples, both in the as-deposited state and after a high-vacuum annealing at 360 ºC. It is also noteworthy that in the as-deposited state no indication of the metallic Co is given by either XRD or TEM techniques, whereas magnetic measurements (particularly, the observation of a significant exchange bias field) evidence its presence.

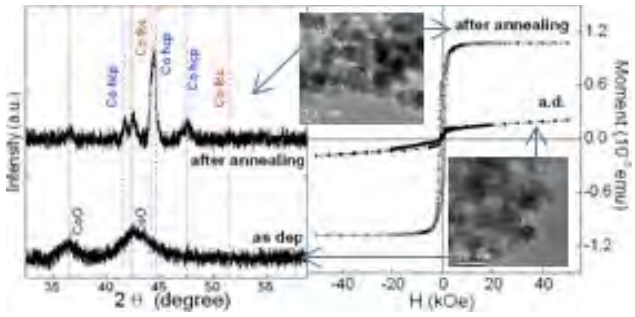

Fig 1. X-ray diffraction patterns, magnetic hysteresis loops and transmission electron microscopy images for a sample, in as-deposited state and after a high-vacuum annealing at 360 ºC.

Finally, the high-vacuum annealing reduction method for cobalt oxide nanoparticles has been proved to be efficient and presents two clear advantages due to its simplicity: a) no need of plasmas [1] or reducing atmosphere with H_2 [2] and b) the relatively low temperatures required. It may then be considered as an alternative to conventional reduction methods to process oxide nanoparticles.

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Interfacial characterization by high resolution depth profiling of undoped and Ga-doped ZnO thin films deposited on a commercial Si (100) solar cell substrate

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The substitutional doping of ZnO with group III elements, such as Ga, has emerged as a way to obtain high quality transparent conducting oxide (TCO). Its high carrier concentration and wide optical band gap energy of above 3.3 eV has made it to be a suitable material in thin film solar cells. The interface between Si and ZnO is a critical part of Si-based solar cells since the conversion efficiency may be profoundly altered by the presence of recombination centers formed at the interface. In previous works, measurements by Transmission Electron Spectroscopy (TEM) and by X-Ray Photoelectron Spectroscopy (XPS) were carried out to determine both the layer and interfacial thickness and the surface chemical composition of these samples, respectively [1]. Nevertheless, this procedure could not be used to analyze the interfacial chemical composition of thicker thin films due to surface nature of this technique. At this point, depth profiling techniques with high depth resolution were performed to allow the interface characterization of ZnO thin films with layer thickness equivalent to those used in commercial Si solar cells. Among the variety of depth profiling methods (Secondary Neutral Mass Spectroscopy (SNMS) is presented as an excellent technique for precise determination of the surface and depth distribution of any film thickness due to the high ion yield and the detection capability at large sputtering depths. SNMS is presented as a powerful tool for the characterization of element distribution and the interface quality of undoped ZnO and Ga -doped ZnO thin films deposited by RF magnetron sputtering on Si wafers. The width of the interlayer between the ZnO film and the Si substrate was influenced by the attained depth resolution and by the thin film surface roughness. The measured thickness of this interlayer was, in both cases, within an order of magnitude of the thin film surface roughness. The quantitative analysis of the interface region revealed an increase of the concentration of the dopant element. The existence of this additional amount at the side nearby the substrate could have a strong effect on the electrical properties of these materials acting as transparent conductive oxides in solar cells devices.

Transient lateral photovoltaic effect in patterned metal-oxide-semiconductor films

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Time dependent transient lateral photovoltaic effect (T-LPE) has been studied in lithographically patterned thin Co films grown over naturally passivated p-type Si (100) substrates. Investigation has been done at room temperature in 21 nm thick, 5 and 10 microns wide and 700 microns long Co films as a function of the position of the laser focused spot with respect to the contacts, pulse frequency (in kHz range) and up to few mW (at wavelength 405 nm or 487 nm) laser power with the spot diameter ranging between 1 and 10 microns. The observed abrupt (faster than in 5 microsecond) change in sign of the T-LPE after the laser is switched off was qualitatively explained by the model which considers redistribution of the life time of non-equilibrium carriers in the electric field due to charged local centres formed during the previous illumination. Exponential relaxation in the inverted T-LPE allows the characterization of the relaxation process as a function of the spot position with respect to the contacts. Numerical simulations satisfactorily reproduce the observed unusual time dependence of the T-LPE.

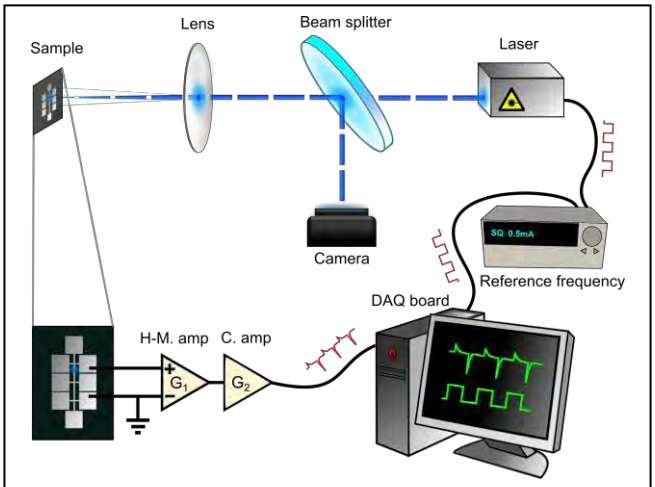

Fig.1. Sketch of the experimental setup: G_1 is a home-made (H-M) preamplifier and G_2 a commercial low noise amplifier. The amplitude-modulated laser beam is focused on top of a thin Cobalt line creating electron-hole pairs in the Silicon substrate. A small signal is generated between the contacts (due to different carrier drifts), amplified and analyzed by a two channel data acquisition board.

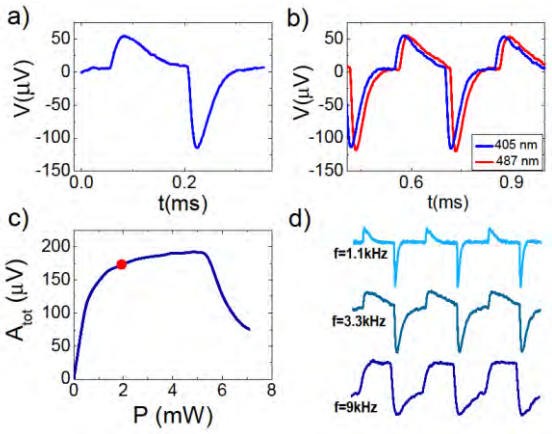

Fig.2. (a) Time dependent T-LPE measured for the 10 μm Co-line. (b) Time dependent T-LPE measured for two different laser wavelengths for the 5 μm Co-line. (c) Power dependence of the signal peak to peak amplitude taken at 3.3 kHz pulse frequency on the 10 μm Co-line. Typically measurements are taken for a laser power indicated by the red dot. (d) T-LPE signals measured with different modulation frequencies for the 10 μm Co-line.

Electrodeposition of Bismuth thin films on n-GaAs

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Bismuth (Bi) is a semimetal with interesting electronic properties for both, fundamental and applied reasons. On one hand, Bi has a large wavelength for electrons in the Fermi level (λ_F = 40-70 nm at room temperature), which allows the observation of quantum size effects (QSE) in nanostructures with at least one dimension in this range [1-3]. On the other hand, Bi surface states are strongly spin-polarized by Rashba effect [4], which could make Bi a material of high impact in spintronics.

For studying QSE in Bi thin films it is compulsory: 1) growth of high-quality films and 2) semiconducting substrates that ensure the existence of a wide Schottky barrier between the Bi film and the substrate [5] in order to avoid current leakage during transport measurements. Taking into account previous studies of Bi growth, electrodeposition has appeared as a suitable technique [6, 7]. This technique consists in the reduction of metallic ions contained in an electrolyte on top of a conductor o semiconductor substrate. Using templates or litographies enable obtaining a wide range of nanostructures (0D, 1D, 2D and 3D).

In this work we present a study of the growth of Bi on n-GaAs substrates with three different orientations: (100), (110) y (111)B. When using single-crystal substrates it must be taken into account its composition but also its surface orientation, as the arrangement of surface atoms it is directly related to the electrode reactivity (figure 1). In addition, we have found some difficulties in the electrodeposition onto n-doped semiconductor substrates due to their electronic properties.

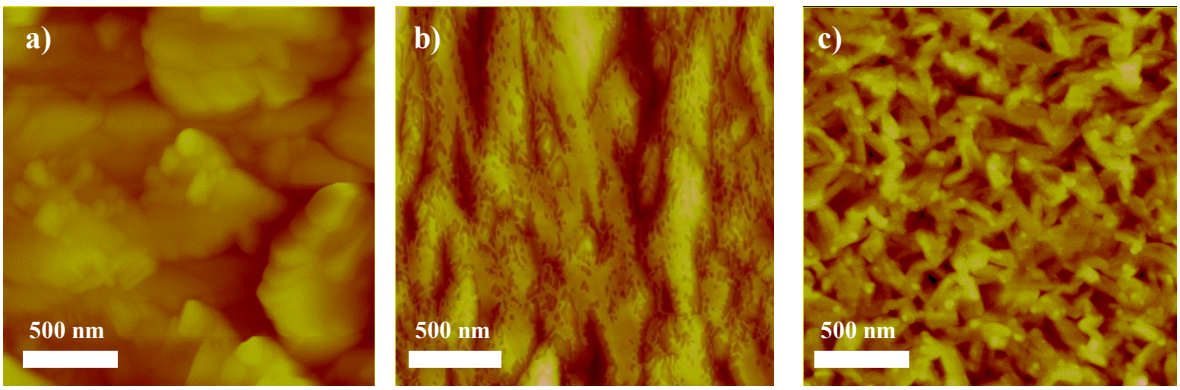

Figure 1. AFM images of 50 nm Bi thin films electrodeposited under same conditions onto n-GaAs substrates with orientation a) (100) b) (110) and c) (111)B.

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Modelización de procesos de inversión de la magnetización mediante corriente inducidos por interacciones de tipo espín-órbita en bicapas metal pesado/ferromagnético

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Experimentos recientes han mostrado que la magnetizacion de una bicapa metal-pesado/ferromagneticocon anisotropia perpendicular se puede invertir mediante una corriente en el plano.A diferencia de lo que ocurre en otras heteroestructuras, como valvulas de espin o uniones de efecto tunel, que requieren la presencia de una segunda capa ferromagnetica y en las que la inversion de la magnetizacion por corriente se debe al llamado *par de transferencia de espín*, en este caso la accion sobre la magnetizacion se debe a *pares de espín-órbita*, llamados asi porque tienen su origen en dicha interaccion. Este tipo de procesos se han estudiado en diversas bicapas como Pt/Co1-3, Ta/CoFeB4, Pt/CoFe5, Ta/CoFe5 o β-W/CoFeB6 y, desde un punto de vista teorico, su explicacion se ha atribuido fundamentalmente a las interacciones de tipo Rashba2,3 o Spin-Hall1,4,5. Algunos autores sostienen que estas interacciones, por si solas, nopueden explicar los resultados experimentales y que otras contribuciones han de ser tenidas en cuenta7.

En esta comunicacion estudiaremos procesos de inversion de la magnetizacion inducidos porcorriente utilizando tanto modelos de tipo *macroespin* como micromagneticos, mediante loscuales intentaremos reproducir cuantitativamente algunos de los resultados experimentalesmas representativos1,2,5. Por un lado, los modelos *macroespin* utilizados hasta el momento han tenido en cuenta unicamente la interaccion de Rashba o la debida al efecto Hall de espin. En nuestro caso tendremos en cuenta ambas interacciones de forma conjunta y, ademas, incluiremos el efecto de las fluctuaciones termicas. De esta forma, mostraremos como la interaccion de efecto Hall de espin es la principal responsable de la inversion de la magnetizacion, si bien los efectos del campo de Rashba no son despreciables. Por otro lado, completaremos nuestro analisis con los resultados obtenidos mediante un modelo micromagnetico que, ademas de los terminos anteriormente citados, incluye la interaccion de *Dzyaloshinskii-Moriya.* Para muestras suficientemente pequenas no existen diferencias significativas en las predicciones de ambos modelos, pero a medida que las dimensiones van aumentando, la interaccion de *Dzyaloshinskii-Moriya* da lugar a la aparicion de estados no uniformes de la magnetizacion, lo cual afecta a las propiedades del ciclo de histeresis.

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Multifunctional Fe-Au heterogeneous thin-films

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Fe-Au heterogeneous thin-films have been deposited by radio frequency (RF) magnetron sputtering [1]. Nanostructural characterization, including transmission and electron microscopy, atomic and magnetic force microscopy and quantitative nanomechanical measurements, shows the granular nature of the thin films, while interferometric measurements reveal a well controlled surface roughness on the order of a few nanometers.

Magnetic and optical properties are of special interest for the implementation of these compounds in the fabrication of multifunctional nanoparticles for biological applications such as hyperthermia treatments, magnetic resonance imaging enhancement, sensors, guided drug delivery to tumour cells etc [2].

By changing the Fe/Au composition, the RF power and the deposition time, a transition from superparamagnetism to ferromagnetic-like behavior can be observed in both magnetization and magnetoresistance measurements. In particular, superparamagnetism is present at room temperature in those alloys with lower Fe content, giving rise to giant magnetoresistance with non hysteretical behaviour. The absence of remanence should prevent particle agglomeration from magnetic interactions, which is one of the main drawbacks for bioapplications.

Optical measurements revealed a maximum in the absorbance coming from the Au. This peak in the optical absorbance makes them suitable as a starting material for the fabrication of Fe-Au nanoparticles with an appropriate optical response for biological applications. By changing the size, shape and embedding medium the maximum absorbance region could be shifted to the near infrared, where biological tissue has high trasmitivity.

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3D vector magnetometry and study of magneto-optical anisotropy in epitaxial Co-films by Generalized Magneto-optical Ellipsometry

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Generalized Magneto-optical Ellipsometry (GME) has emerged in the last decade as a methodology to characterize magnetic materials with a high degree of precision by utilizing the magneto-optical Kerr effect [1]. Compared to other magneto-optical characterization methods based on the same effect, GME has two key advantages: it can measure both the optical and magneto-optical constants, and it allows full vector magnetometry, all with one simple experimental set-up. Recently, we reported on further improvements of GME that enabled unprecedented precision and reliability [2]. The technique has already been successfully employed in the study of diverse magnetization reversal processes, including measurements of the magnetization orientation using 2D vector magnetometry [3]. However, even if some works have suggested the possibility to perform quantitative 3D vector magnetometry using GME [4], actual measurements have not been demonstrated so far.

Here, we show for the first time that we are able to extract the field dependent evolution of all three magnetization components, which we studied for the reversal processes of epitaxial Co and Co-alloy based thin films and multilayers. In order to do so, we exploit the different symmetries of the longitudinal, transverse and polar Kerr effect with respect to the relative polarizer/analyzer orientation, which allows us to separate each of the magnetically induced contributions to the reflection matrix elements.

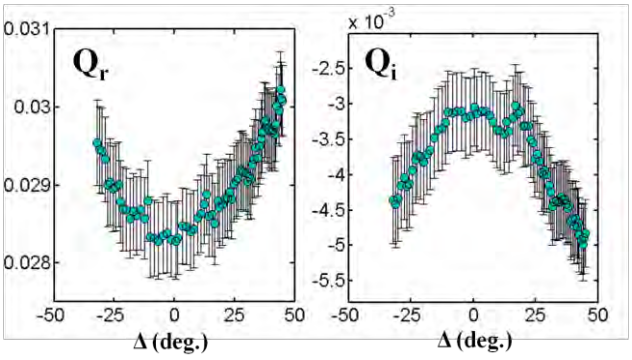

Fig 1. Dependence of the magneto-optical coupling constant $Q = Q_r + iQ_i$ on the magnetization orientation with respect to the in-plane crystallographic *c*-axis of Co (easy axis) at the wavelength $\lambda = 635$ nm. The magneto-optical constant shows a marked anisotropy as the magnetization is driven away from the easy axis.

By means of this full vector magnetometry capability, our unique methodology also enables us to investigate magneto-optically active materials that show both optical [5] and magneto-optical anisotropy at the same time. Thus, we have experimental access to study the relation between these anisotropies and other material parameters as well.

Finally, we also utilize this methodology to study the optical, magneto-optical and the magnetic behavior of wedge shaped Co/Ag/Co multilayer structures.

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Multiple Andreev reflection and critical current in topological superconducting nanowire junctions

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Fermions that are their own anti-particle, known as Majorana fermions (MFs), were originally predicted in particle physics, however, it is in condensed matter systems that their realization is close to be reality. In recent years the interest in such exotic (condensed matter) excitations has increased vastly, since they exhibit non-abelian statistics and therefore can be used in topological quantum computation.

Semiconducting nanowires (NWs) with a strong spin-orbit (SO) coupling in the proximity of s-wave superconductors and in the presence of an external magnetic field are a promising platform to study Majorana fermions in condensed matter physics. Although there have been many experimental proposals in oder to detect such exotic excitations, it is still missing a fully agreement between the theory and the experimental realizations.

We study transport in voltage-biased Superconductor-Normal-Superconductor (SNS) junctions made of NWs with strong SO coupling, as it transitions into a topological superconducting phase for increasing Zeeman field B. We propose the multiple Andreev reflection (MAR) current in voltage-biased SNS junctions, I_{dc}, as an alternative, flexible experimental probe to study the topological transition of junctions made of semiconducting NWs. By employing Keldysh-Floquet theory and the Recursive Greens functions method it is computed the MAR current I_{dc} through a biased SNS junction as a function of a bias voltage V and junction transparency (at small, intermediate and full transparency regimes). Despite the absence of a fractional steady-state ac Josephson current in the topological phase, the MAR current at different junction transparencies is particularly revealing. It exhibits unique features related to topology, such as the gap inversion, the formation of the Majorana bound states and fermion-parity conservation. Moreover, we have found that the critical current I_c, which remarkably does not vanish at the transition where the system becomes gapless, provides direct evidence of the topological transition.

Although we have focused here on the simplest case (single-band, short junction limit) we expect the main features of the topological transition to remain robust under more general conditions. We therefore believe that experiments along the lines discussed in this work could provide the first unambiguous report of a topological transition in NWs, and the emergence of Majorana bound states.

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Theory of magnetic anisotropy renormalization induced by exchange coupling

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Here we show that the magnetic anisotropy of a quantum magnetic system, a property that controls its suitability for use in magnetic data storage devices [1], is controlled by the interaction with the electrons of a nearby conductive electrode. The theoretical prediction is confirmed by scanning tunnelling microscopy and spectroscopy of Co atoms deposited on a Cu_2N substrate [2]. The observed variations can be accounted for by both, a simple treatment of the Kondo exchange coupling based on perturbation theory [3,4], and a numerical approach based on the one crossing approximation [2]. In particular, this system constitutes one of the few examples in nature where the renormalization of the energy levels induced by coupling to the environment and not just the excited-state finite lifetime is observable experimentally.

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Superexchange blockade of triple quantum dots

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Quantum mechanics allows for superpositions of indirectly coupled states even if the intermediate states are far in energy. This is done via superexchange: higher order transitions in which the energetically forbidden intermediate states are only virtually occupied. Such long range transitions are central to the theory of the chemical bond and are present in chemical reactions, spin phenomena in the solid state, quantum optics, and even biological processes. Increased interest has appeared recently in the context of quantum information processing aiming at the low dissipation transfer of quantum states or the operation of two distant qubit gates.

Semiconductor quantum dot arrays offer a fully tunable possibility to manipulate the coherent coupling of quantum states. The recently achieved control of triple quantum dots open the possibility to investigate phenomena relying on quantum superpositions of distant states mediated by tunneling. Here we investigate the minimal system with long range superexchange interactions affected by spin correlations. It requires three sites and two electrons. Superexchange is responsible for the indirect coupling of the two outer quantum dots, mediated by virtual transitions through the middle one. Evidences of such transitions have been recently reported in the form of sharp current resonances at the degeneracy points of states with left-right symmetric charge distributions [1,2]. The transition can take two paths: two electrons in different dots tunnel simultaneously [1] or a single electron tunnels twice [2], as sketched in Fig 1. The effect was confirmed by real time charge detection of left-right higher order tunneling in two electron configurations [3]: resonant transitions between $(N_1,N_2,N_3)=(1,1,0)$ and $(0,1,1)$ configurations -N_I being the number of electrons in each quantum dot- are detected where the intermediate states, (0,2,0) and (1,0,1), are not occupied.

We are interested in a configuration where the two different paths with (1,0,1) and (0,2,0) virtual states are possible and lead to quantum interference. Remarkably, we find conditions where the destructive interference of these transitions completely cancels the transport, what we call superexchange blockade [4]. The system thus work as a one dimensional interferometer.

Spin correlations due to the Pauli exclusion principle also play an essential role by avoiding virtual transitions through the (0,2,0) state whenever the two separate electrons form a spin triplet. This effect, known as spin blockade, leads to the suppression of certain resonances whose observation give a measure of spin decoherence times.

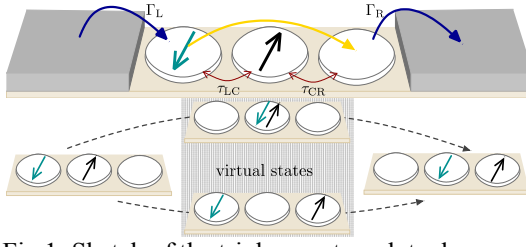

Fig 1. Sketch of the triple quantum dot where transport is dominated by superexchange transitions. Intermeditate states are only virtually occupied

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Spin configurations of individual $Fe_{3-x}O_4$ nanoparticles

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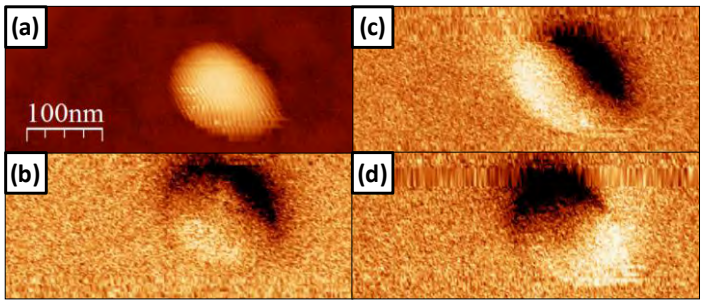
Magnetic nanoparticles (MNPs) are attractive materials object of many studies in the recent past years due to their potential applications in nanotechnology, such as in data storage, magnetic resonance imaging, catalysis or environmental remediation **[1]**, and in biomedicine, including biomolecule detection, magnetic hyperthermia or targeted drug delivery **[2]**. Not only reliable and reproducible methods of nanocrystal synthesis are of key importance in order to obtain uniformly sized MNPs but also high resolution characterization techniques with accurate magnetic sensitivity are necessary to unveil their domain configurations and magnetization reversal processes.

In this work, we present synthesis **[3]** and magnetic domain characterization of $Fe_{3-x}O_4$ nanoparticles – ranging from 15 to 100 nm – by organic decomposition methods, using iron (III) acetylacetonate as precursor and decanoic acid as surfactant and stabilizer. Domain structure of clusters and individual nanoparticles were obtained by magnetic force microscopy (MFM) under variable in-plane or out-of-plane magnetic fields. In addition, micromagnetic simulations were performed with the OOMMF code to help with the interpretation of the sometimes non-trivial contrast in MFM images.

Furthermore, some hints are provided about artifacts that might be present when measuring magnetic nanoparticles with MFM, such as influence of the topography and/or electrostatic overlap **[4]**. Their contribution should be taken into account for a correct interpretation of MFM data.



(a) Topography of a single $Fe_{3-x}O_4$ nanoparticle (d≈30 nm). MFM images show different orientations of a single domain (b) at remanence and under horizontal fields of (c) + 23 mT and (d) -23 mT.

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Low-temperature specific heat of extremely stabilized glasses: do tunneling states persist or disappear?

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We have investigated how extreme thermal histories in glasses can affect their universal properties at low temperatures. With such an aim, we have employed calorimetric techniques to investigate this phenomenology both around the glass transition and at low temperatures, where the universal excess excitations in glasses above the Debye-expected contribution appear. In particular, we have studied two materials which allow us to access highly-stable glassy states, as well as their corresponding conventional glasses, in two completely different ways: (i) amber[1,2], the fossilized natural resin, which is a glass which has experienced a hyperaging process for about one hundred million years; and (ii) ultrastable thin-film glasses of indomethacin[3] (an organic molecule commonly used in pharmaceuticals), prepared by physical vapor deposition at temperatures around 85% of its glass-transition temperature.

Specifically, we have studied 112 million-year-old amber samples from El Soplao (Cantabria, Spain). Specific heat C_p measurements of pristine, partially- and fully-rejuvenated samples were conducted in the temperature range $0.07\text{K} < T < 30$ K, as well as around its glass-transition temperature $T_g \approx 150$ºC. A modest increase of the boson-peak height (in C_p/T^3) with increasing rejuvenation was observed, that can be related to a corresponding increase of the Debye coefficient. The amount of two-level systems, assessed at the lowest temperatures, was however found to be exactly the same for the pristine *hyperaged* amber as for the subsequently rejuvenated samples.

On the other hand, conventionally prepared thin films of glassy indomethacin exhibit the usual linear term in the specific heat below 1 K ascribed to the universal two-level systems in glasses. Nevertheless, we have observed an unexpected suppression of these two-level systems in the ultrastable glass.

By comparing both highly-stable kinds of glass, we conclude that the disappearance of the tunneling two-level systems in ultrastable thin films of indomethacin is due to the quasi-2D and anisotropic behavior of this glass, what supports the idea of a phonon-mediated interaction between two-level systems, as proposed by Yu and Leggett[4].

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Quantum Capacitance and Electromigration in atomic-sized Contacts

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In recent years electron transport through metallic contacts at the nanoscale has been studied theoretically and with experiments. The most studied quantity is the current along with its derivatives. However, this is not the only quantity that can be measured. Capacitance also gives valuable information about the electronic and structural properties of the nanocontacts. We are interested here in the Quantum Capacitance which depends on the density of states and measures the quantum contribution to the capability of a device to accumulate electrons. This quantity depends of the chemical nature, i.e., of the available atomic levels of the material. It also depends of the energy with which electrons are injected. Therefore, it has a quantum mechanical origin in contrast to the purely electrostatic one [1].

We used ab-initio calculations based on DFT methods and the Green's function formalism to simulate such systems. To introduce non-equilibrium conditions, we apply an external bias voltage, at which electrons are injected.

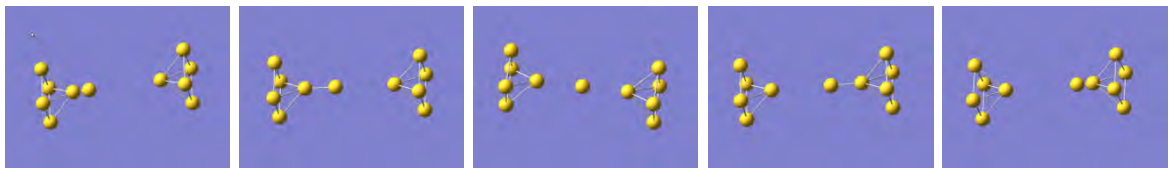

Fig. 1: Simulation of Gold atom electromigration between two contacts under applied bias voltage.

We also studied how the charge distribution affects the nonequilibrium induced forces on the atoms forming the junction. This allows us to explain the transfer of atoms between the metallic electrodes mediated by the bias voltage. This phenomenon is called electromigration.

Among the simulated systems, there are contacts from different metals. Non-voltage-symmetric charge distributions and current-voltage characteristics emerge of our calculations. This is a result of the absence of electron-hole symmetry. The distinctive DOS corresponding to each of the metals is determinant in the capacitance, as well as other transport properties.

If an atom moves between the two biased contacts, there arise forces occurring on the atom. These appear due to the nonequilibrium charge distribution [2]. The free energy that describes an out of balance problem, loses the symmetry corresponding to equilibrium. This leads forces that can determine a preferred direction for the electromigration of the atoms.

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Modification of the Magnetic Properties of $Y_2Ru_2O_7$ by Zn/Mg Doping on the Y site

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Geometric magnetic frustration occurs in materials when, due to the topology of the lattice, the system is unable to reduce its total energy by minimizing the interaction energy between competing interacting degrees of freedom.[1] An excellent example of this type of frustration is afforded by materials which adopt the cubic pyrochlore structure, with general chemical formula $A_2B_2O_7$, where both the A and B site ions form an interpenetrating network of corner sharing tetrahedra.[2] At the classical mean field level spin configurations that have zero net moment on all tetrahedra form a degenerate lowest-energy manifold and therefore do not develop long-range order for T>0 K. As a result the low-temperature properties are determined by sub-leading interactions, thermal and/or quantum fluctuations, leading to the formation of, for example, spin glasses, spin liquids, or magnetoelastically induced Neél order.[3, 4]

Within this family of materials, the ruthenium pyrochlores, $A_2Ru_2O_7$, display a multitude of interesting properties, due to the fact that ruthenium can be either in the 4+ or 5+ oxidation state. For example, in the case of Ru^{4+}, $R_2Ru_2O_7$ (R= Y, rare earths) are insulating and show spin-glass/long-range order transition, while $Bi_2Ru_2O_7$ (isoelectronic to $Y_2Ru_2O_7$) is a Pauli paramagnet.[5-9] It is thought that the insulator-vs-metal behaviour in this family of materials can be explained in terms of the Mott-Hubbard mechanism of electron localization, with the metallic compounds having greater Ru-O-Ru bond angles and shorter Ru-O bond length than the insulating ones.[10] Experimental work has been reported on several solid solutions, such as $Y_{2-x}Bi_xRu_2O_7$ and $Bi_{2-x}M_xRu_2O_7$.[11, 12] Here we expand on these studies by investigating the effect on the physical properties of $Y_2Ru_2O_7$ when substituting Y^{3+} by either Mg^{2+} or Zn^{2+}.

X-ray diffraction reveals that in both cases the solid solution exists up to x= 0.2. Susceptibility measurements show that the magnetic transition reduces with increasing Mg/Zn content. This is consistent with what has been observed for $Y_{2-x}Ca_xRu_2O_7$ and can be either due to oxygen non-stoichiometry ($Y_{2-x}(Zn/Mg)_xRu_2O_{7-\delta}$) or Ru becoming mixed valent (Ru^{4+}/Ru^{5+}).[11] In order to determine which of these two scenarios is correct we have performed both muon and neutron diffraction experiments on $Y_{1.8}Zn_{0.2}Ru_2O_7$. Results of these measurements will be presented here.

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The role of orbital differentiation in the magnetic state of iron superconductors

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In iron high Tc superconductors, superconductivity emerges when an antiferromagnetic state is suppressed by doping, applying pressure, or by isovalent substitution. In most of the cases, the parent compound is metallic, shows columnar magnetic ordering, and is anisotropic in the a-b plane. The Fe atoms are in a square lattice and in tetrahedral coordination with out-of-plane As, P, Se, or Te. The origin and nature of the magnetic state in these materials is still under debate. In particular, there is a lively discussion on the strength of the interactions whose outcome is crucial for the determination of the superconductivity mechanism.

One of the important characteristics of Fe superconductors from the electronic structure point of view is the fact that all five 3d Fe orbitals contribute to the bands close to the Fermi energy. In principle, interactions can affect each orbital differently. In this direction, the idea of an orbital selective Mott transition has been discussed [1] and different renormalizations of the orbitals have been found [2]. Starting from a tight-binding model which includes all the Fe 3d orbitals, and takes into consideration the geometry of the tetrahedra through the indirect Fe-As-Fe hoppings [3], we have studied the magnetic state of iron superconductors [4,5,6]. We use both mean-field calculations and strong coupling arguments to analyze the role of the different orbitals and the effect of the interactions on their reorganization in the magnetic state. We find that the degree of localization of the orbitals is a consequence of the delicate interplay between kinetic energy and superexchange gain. From our model we can infer that the orbital differentiation arises as a result of the non-trivial anisotropies in the hoppings and the superexchange interactions that result from the tetrahedral coordination [7].

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Specific heat of $La_{1-x}Sr_xMnO_3$ and $La_{1-x}Ba_xMnO_3$ revisited

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In this work we present specific heat (c_P) measurements of $La_{0.7}Sr_{0.3}MnO_3$, $La_{0.8}Sr_{0.2}MnO_3$ and $La_{0.7}Ba_{0.3}MnO_3$. From the analysis of our low temperature results ($T < 20$ K) we conclude the existence of a spin-wave contribution (c_{sw}) for the three materials studied. Besides of that, a thorough analysis of the medium and high temperature data (20 K < T < 390 K) has allowed us to separate the magnetic contributions to c_P in the whole experimental temperature, as well as to evaluate the total magnetic entropy developed at the Curie temperature T_C. Contrary to different previous reports, our values are similar to the theoretical predictions for the S=3/2 for the Mn ion (figure 1, casting some doubts of interpretations of specific heat measurements in terms of *missing entropy* [1-3], related with peculiarities of the magnetic phase transition in manganites, as short range correlations above T_c or the existence of spin fluctuations.

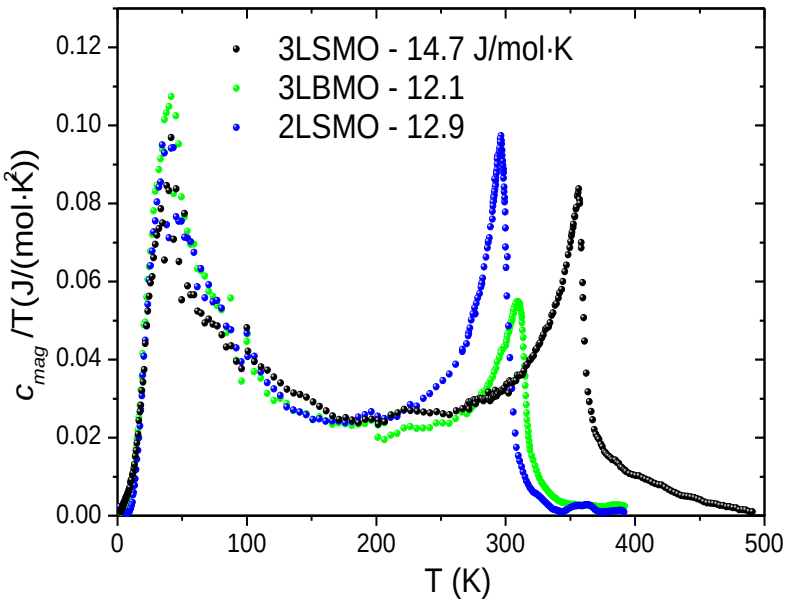

Figura 1. c_{mag}/T vs. T para los tres materiales estudiados en este apartado. La entropía magnética total calculada a partir de estos datos es de 14.7, 12.1 y 12.9 J/mol·K para 3LSMO, 3LBMO y 2LSMO respectivamente

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From adiabatic to adiabatic regime in periodically driven p-wave superconductors

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P-wave superconductors possess a topological invariant (winding number) which implies the existence of localized end-states. The effect of an AC variation of the chemical potential is studied using Floquet theory [1], including different driving frequency regimes and the corresponding topological invariants. In the high frequency regime the winding number takes non trivial values as 1 or -1 depending on the ac and dc components of the chemical potential. When the frequency is lower, the system can have end-states associated with the coupling between Floquet bands [2]. This implies that the winding number can have larger values than in the high frequency regime. We study the behavior of these end-states with a larger winding number [3] and, finally, the adiabatic regime is explored.

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Millikelvin Scanning Tunneling Spectroscopy on the superconductor $Ca(Fe_{0.965}Co_{0.035})_2As_2$.

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We have studied the superconducting iron pnictide compound $Ca(Fe_{0.965}Co_{0.035})_2As_2$ using millikelvin scanning tunneling spectroscopy. High quality single crystals were grown using solution growth techniques. Topographic and spectroscopic images were performed at 30 mK using STM/S (Scanning Tunneling Microscopy and Spectroscopy). Clean and large flat areas are found over the surface. Our images, made at 30 mK, show surface atomic reconstruction observed previously at 4.2 K [1] and further features pertaining the superconducting properties of this compound.

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Quantum Coherent Transport through AC Driven Quantum Dots Arrays

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Recently, complex spin qubit circuits such as triple quantum dots are being developed. In these systems in serial configuration, bipolar spin blockade has been demostrated (1). Spin blockade is a consequence of the Pauli exclussion principle and occurs when two neighbor dots have electrons with parallel spins. Then the transfer of one electron to its neighbor dot is forbidden and the current drops. Furthermore, recent works (2,3) have shown that in triple quantum dots two distant sites can be tunnel-coupled directly. The coupling is mediated by coherent superpositions such that a single charge oscillates coherently between the outer sites of a triple dot array without passing through the middle. Such states have been invoked theoretically for possible applications such as spin bussing or quantum rectification.

In the present work we discuss long range quantum transfer through coherent superpositions in triple quantum dots in series where the system is driven by an AC voltage. In particular, we will consider up to two extra electrons in the system and we will discuss coherent superpositions giving rise to transport between the edge dots and the role played by the ac field. We analyze as well the presence of dark states. coming from destructive interference of different electron paths and the effect of spin flip , on the dark state superposition.

Controlling long-distance quantum correlations in quantum dot arrays is central to quantum computation and simulation. The long-distance coupling significantly improves the prospects of fault-tolerant quantum computation using quantum dot arrays, and opens up new avenues for performing quantum simulations in nanoscale devices.

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Scanning Tunneling Microscopy at Low Temperatures and Vectorial Magnetic Fields.

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We present a Scanning Tunneling Microscope (STM) set-up capable to measure at very low temperatures under vectorial magnetic fields. The system consists of a STM installed in a dilution cryostat with base temperature below 50 mK, inserted within a superconducting magnet which allows us to generate magnetic fields of the order of several Tesla in any spatial direction. We study the Charge Density Wave (CDW) variations with temperature in the superconductor $NbSe_2$. We also study the vortex lattice dependence with the angle of the applied magnetic field in the same material. The vortex core in this compound exhibits a six-fold star shape which is a consequence of its anisotropy in the superconducting properties. Here, we will discuss the evolucion of the vortex core states as a function of the azimuthal orientation of the magnetic field respect to the atomic crystalline lattice.

Simultaneous magnetic order of Mn and Co in $Mn_{0.85}Co_{0.15}WO_4$ by resonant magnetic x-ray scattering

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$MnWO_4$ is a frustrated type-II multiferroic where magnetic and ferroelectric orders are found to coexist and mutually interact. At low temperatures (~7.5-12.5 K), the development of an incommensurate (ICM) magnetic Mn cycloidal spin structure (AF2 phase) is responsible for the appearance of a net electric polarization along the crystal *b*-axis [1-3].

A small partial substitution of Mn by Co tends to stabilise AF2 down to the ground state. For more than ~ 7.5% Mn ions replaced by Co the ground state corresponds to a new ICM phase, defined as AF2' or AF5 [4]. For a larger doping the presence of Co drives the appearance of a commensurate (CM) antiferromagnetic collinear phase, called AF4.

In $Mn_{0.85}Co_{0.15}WO_4$, AF4 is observed in the interval $10< T< 17$ K. We have performed resonant magnetic x-ray scattering (RMXS) with soft x-rays (Mn, Co $L_{2,3}$ absorption edges) on $Mn_{0.85}Co_{0.15}WO_4$ to independently analyze the magnetic order in Mn and Co ions. A full polarization analysis of the incident and scattered x-rays permits us to provide an accurate picture of the order of Co and Mn magnetic moments in the CM AF4 phase. Co spins turn out to be antiferromagnetically ordered following the single-ion anisotropy axis as found in $CoWO_4$ [5]. Co magnetic anisotropy energy strongly influences Mn spins alignment direction, which was studied independently. We discuss RMXS results in the frame of the complex phase diagram of $Mn_{1-x}Co_xWO_4$ multiferroics.

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Statistical velocity distribution of single domain wall in magnetic microwires

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The dynamics of domain wall, DW, motion in magnetically bistable amorphous microwires has been extensively studied in connection to their technological potential as well as for fundamental micromagnetic and dynamics research [1,2]. Particularly, the controlled motion of single DW has been recently investigated [3,4].

In the present study we introduce a statistical study of the single DW dynamics in amorphous $Fe_{72.5}B_{15}Si_{12.5}$ glass-coated microwire performed over thousand events. The microwire (19.3 μm metallic-nucleus diameter, coated by 13.5 μm thick glass-layer) is characterized by a large single-domain core longitudinally magnetized having a switching field of 40 A/m, ideal for magnetization reversal study through single DW. For this work, a special set-up was designed where the DW movement is induced by an external square-wave AC (11 Hz to 101 Hz frequency) main magnetic field parallel to the wire axis.

The DW velocity is recorded by two pairs of pick-up coils equidistantly located, before, v_1, and after, v_2, a 4 mm long local field coil, L_c, used either in parallel or antiparallel configuration to the main field to induce local changes in the DW dynamics. Two scenarios are considered under a small (40 A/m) main field: i) a "standard" single DW depinned from one end of the wire propagates to the other end passing through the interference caused by the local field, H_L, at the L_c position (the statistical fluctuations of velocity v_2 are shown in the figure for H_L=0 and antiparallel local field, H_L =73 A/m), and ii) a pair of DWs "injected" at Lc are allowed to propagate to both ends. The statistical difference between v1 and v2 is discussed for both H_L configurations in terms of H_L strength and direction. The different dynamic of walls depinned from the ends and those nucleated and propagated from the centre is also presented and discussed.

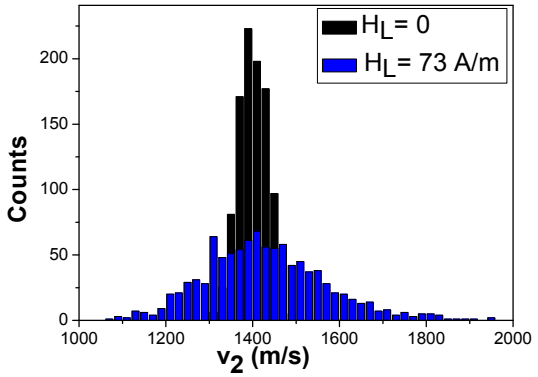

Fig 1. Statistics of v_2 velocity under H_L=0 and antiparallel local field, H_L =73 A/m, for the standard single DW propagating in the circular magnetic microwire under small main homogeneous field.

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4f metals: exploring Gadolinium nanocontacts

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The study of electron transport in conducting materials at the nanoscale can be carried out by using Scanning Tunneling Microscope (STM) and Mechanical Break Junction techniques (MBJ) [1]. At such scales, Kondo effect vanishes the magnetic properties of the 3d transition metals Fe, Co and Ni [2]. The 4f rare earth metals are an interesting aim of study because of their strong magnetic properties among other things. At our laboratory we have measured gadolinium with a STM. In the spectroscopy measurements of this material we perceive a set of features that could be related to its magnetic properties. The interplay between the $4f^7$ and $5d^1$ orbitals at Gd drives us to pose the mechanisms that are involved in the electronic transport properties of these systems.

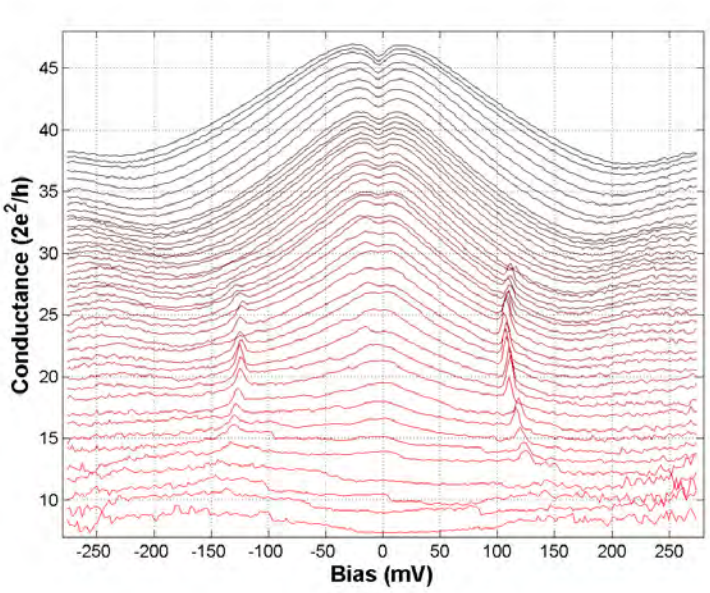

Fig 1. Gd>Gd measurements taken using STM at cryogenic conditions.

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Exploring molecular magnetism on the surface of a superconductor

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Magnetism and superconductivity are phenomena that cannot simultaneously exist in the same region of a material: weak applied magnetic fields are expelled from the superconductor, while strong magnetic fields destroy the superconducting properties. An interesting playground to study the interplay between both phenomena are magnetic impurities in a superconductor. They can either destroy locally the superconducting state or be fully screened, depending on the specific details of how the local magnetic moment interacts with the Cooper pairs.

Using scanning tunnelling spectroscopy at low temperatures and ultra-high vacuum, we investigate these interactions at the level of single paramagnetic molecules on a superconducting lead surface. For the case of sizeable coupling between magnetic moment and quasiparticles at the lead substrate, we observe localized states in the superconducting energy gap [1,2,3]. These bound states reflect the weakening of the superconducting paring [4] and allows us to track the pair-breaking process. From our results we are able of resolving the delicate balance of interactions of the magnetic impurity with either Cooper pairs or normal electrons. While the former leads to the rupture of the superconducting state, the later screens the magnetic moment of the impurity via the Kondo effect. The balance turns out to be sensitive to the atomic scale environment, which thus determines the resulting ground state of the system [4].

By simply modifying the molecular functionalisation interactions with the superconducting environment can be tuned, allowing us to detect spin excitations [5] in molecules retaining their paramagnetic state on a superconducting substrate. An interesting outcome is that the lifetime of excited states amounts to a few nanoseconds, much larger than on normal metal surfaces [6]. This is interpreted as due to the depletion of electronic states within the superconducting energy gap at the Fermi level, which prohibits pathways of energy relaxation into the substrate.

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Josephson current in topological superconducting nanowires with Majorana fermions

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In last years the interest on Majorana fermions has increased due to their topological nature that protects them against sources of decoherence, one of the main problems nowadays in quantum computation. Indeed, these exotic excitations exhibit non-Abelian statistics that could be used to implement topological quantum computation.

It was predicted that p-wave superconductors host Majorana fermions since they realize topological phases. One can mimic such p-wave physics by considering semiconducting nanowires (NWs) with a strong spin-orbit (SO) coupling in the proximity of s-wave superconductors and in the presence of an external magnetic field. The Zeeman field drives the system into the topological phase where Majorana fermions emerge at the ends of the nanowire.

In this work, we study transport in Superconductor-Normal-Superconductor (SNS) long (and short) junctions made of NWs of finite length with strong SO coupling, as it transitions into a topological superconducting phase for increasing Zeeman field B. By employing exact diagonalization the Andreev levels are calculated and then we investigate their evolution into Majorana bound states. Moreover, the Josephson current (or supercurrent) is calculated in the transparent regime, where the Andreev levels play an important role. By increasing the Zeeman field, the system experiments the closing and reopening of the topological superconducting gap that leads to the topological phase with four Majorana fermions. Calculations on the critical current that provides an evidence of the topological transition are also presented, and suggest that experiments in this regard should be performed in order to detect such exotic excitations.

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Beyond room temperature exchange-bias stabilization in core-shell Co-CoO nanoparticles dispersed in a NiO matrix

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One of the strategies that have been suggested in order to "delay" the appearance of the so-called *superparamagnetic limit* in magnetic storage technology is the effective increase of particle anisotropy provided by its exchange coupling with an antiferromagnetic (AFM) material [1]. This effect has been previously demonstrated in the archetypical Co-CoO system, where, however, the exchange-bias driven stabilization is restricted to temperatures below room temperature. In thin layer geometry, stabilization beyond room temperature has been achieved by combining the properties of CoO and NiO (with lower anisotropy but higher Néel temperature than CoO) [2].

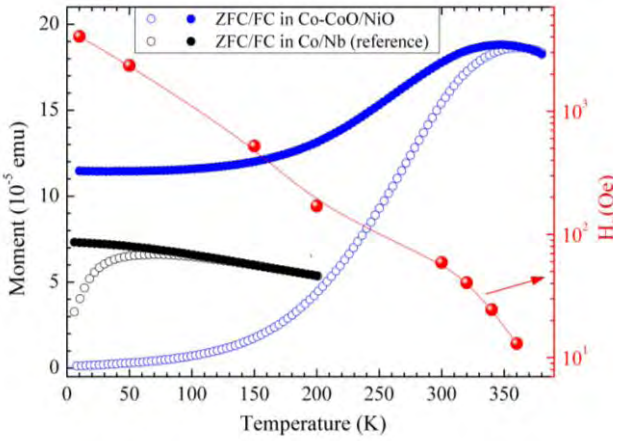

Fig. 1. Left axis: field (FC) and zero-field (ZFC) cooled magnetization curves measured for identical Co particles either dispersed in a Nb matrix (black symbols) or after partial oxidation followed by dispersion in a NiO matrix (blue symbols). Right axis (red): temperature dependence of the exchange-bias field (the line is a guide to the eye).

In this contribution we present similar results (as shown in Fig. 1) in *particle* geometry, where pre-formed Co particles (prepared by gas-phase condensation as in Ref. 3) are partially oxidized in the deposition chamber (to form core-shell Co-CoO particles) before being buried in a sputtered NiO matrix. Co particles condensed using the same cluster-source parameters (yielding a particle diameter ≈ 5 nm) were also dispersed in a niobium matrix for comparison. The observed large stabilization effect reaches beyond room temperature, with the blocking temperature of the Co-CoO/NiO system (≈ 350 K) roughly coinciding with the onset temperature of the exchange-bias field, which confirms that this effect is due to the effective exchange-coupling of the Co cores with either both CoO and NiO (allowed by a very thin CoO shell) or with a hybrid $Co_xNi_{(1-x)}O$ phase formed at the interface between the particles and the NiO matrix.

DP Marques acknowledges financial support from the Brazilian CNPQ.

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Direct observation of backscattered polariton condensates in a quasi one-dimensional microcavity

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We discuss the effects of inter-particle interactions on the propagation of a Bose-Einstein-like polariton condensate in a quasi one-dimensional semiconductor ridge micro-cavity [1,2], studied by time-resolved optical spectroscopy in real- (Fig. 1(a)) and momentum(**k**)-space (Fig. 1(e)). By filtering the emission in real- (Fig. 1(b)) and **k**-space (Figs. 1(g,h)) [3], we monitor the polaritons backscattered by defects in the microcavity.

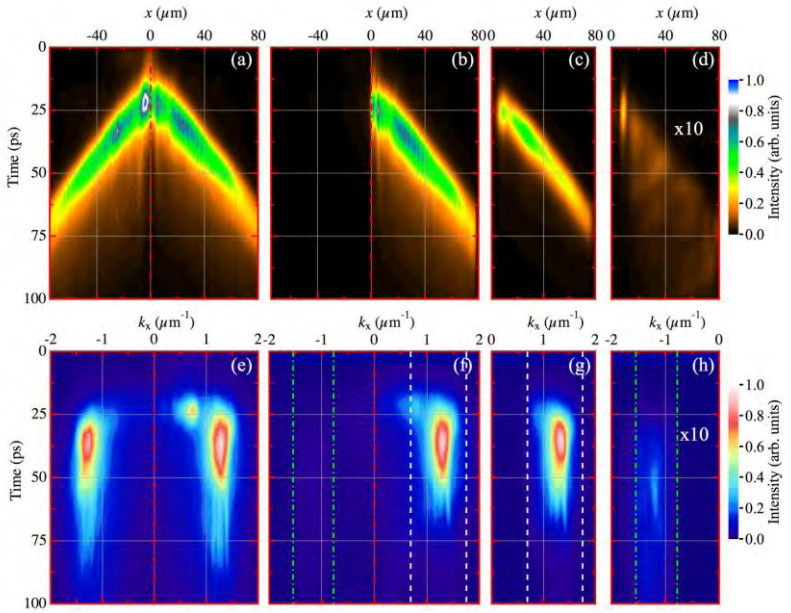

Fig. 1. Time resolved real-/momentum-space distribution of the polariton wave trains emission under the following filtering conditions: (a)/(b) no-filtering, (b)/(c) filtered real-space for $x<0$, (c)/(g) filtered real- and momentum-space for $x<0$ and ($k_x<0.8$) & ($k_x>1.6$) μm^{-1} and (d)/(h) filtered real- and momentum-space for $x<0$ and ($k_x<-1.6$) & ($k_x>-0.8$) μm^{-1}. Polariton emission in panels (d,h) is multiplied by a factor x10. Intensity is coded in a linear, false color scale.

A quantitative analysis obtains the populations of incident ($k_x>0$), Figs. 1(c,g) and backscattered polaritons ($k_x<0$), Figs. 1(d,h), in the ultrafast propagation dynamics. The spatial overlap of these counter-propagating condensates yields the coherent interference modulation of the real-space emission intensity, shown in Figs. 1(a,b). These results on polariton scattering in a quasi-frictionless flow of condensates are very relevant for the fabrication of integrated polariton circuits with high transmissivity [4].

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Integrated photonic devices driven by coherent surface acoustic phonons

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One of the major challenges for integrated photonics, as compared with electronics, is the ability of controlling and manipulating the photons within small dimensions. Because of that, the search for solutions that allow devices that are the same time fast, compact, efficient, low-cost, externally controlled, and compatible with integration technology is of paramount importance. A promising approach consists of using a strong population of coherent surface acoustic phonons (in the form of a surface acoustic wave, SAW) to modulate multiple optical waveguides (WGs) through the acousto-optical effect [1]. In this way, it is possible to address multiple devices using only one SAW, due to its very large phase coherence. This provides an excellent compromise between speed and size. In this contribution, we will address the design, fabrication, and characterization of a tunable photonic modulator consisting of two 180º-dephased output waveguide channels, driven by a surface acoustic wave in the GHz frequency range built on (Al,Ga)As [2]. Odd multiples of the fundamental driven frequency are enabled by adjusting the applied acoustic power. A good agreement between theory and experimental results is achieved. The device can be used as a building block for more complex integrated functionalities and can be implemented in several materials platforms.

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Polarization switching in microcavity polariton condensates

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Microcavity exciton-polaritons are composed quasi-particles arising from the strong coupling between confined photons by a Fabry-Perot (FP) cavity and excitons created in a quantum well, embedded in the antinode of the optical field inside the FP [1]. They present a bosonic behavior, within the limit of a diluted gas, and their excitonic component allows them to interact with each other: For quasi-resonant excitation it is possible to generate parametric scattering processes when two polaritones, created at the inflection point of the lower polariton branch, scatter into the signal and idler states, in an optical parametric oscillation (OPO) process that conserves energy and momentum [2]. In this manner, condensates of polaritones can be created, which show superfluidity [3] and fascinating coherent properties [4].

We studied a hybrid system where a 2D and 1D systems co-exist allowing us to investigate simultaneously the polarization properties of both condensates created in an OPO process. Remarkable differences in their light emission appear when the polarization plane of the excitation laser is changed: while the 2D condensate emits polarized light rotated 90 degree with respect to the polarization of the excitation laser [5], the 1D condensate presents a switching behavior between two highly linearly polarized state. Two complementary models, based on semi-classical Boltzmann kinetic equations and on the Gross-Pitaevskii equation, respectively, obtain an excellent agreement with the experimental results, providing a deep insight into the mechanisms responsible for the polarization switching.

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Characterization of amorphous and porous silicon coatings by (S)TEM and EELS

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In recent papers [1,2] we presented a new bottom-up methodology for the production of amorphous and porous SiO_xN_y and Si coatings deposited by rf magnetron sputtering of silicon targets. In the case of silicon this new approach allows the production of a closed porosity in contrast to the previously most common way of chemical etching in HF-based solution, which leads to open porosity. By the choice of the atmosphere, Argon or Helium, we could produce dense or porous coatings with refractive indices of 4.75 and 3.75 respectively [1]. It has been shown how the use of He as process gas gives rise in the case of Si to this singular microstructure of closed pores, filled with the deposition gas and aligned on the coatings' growing direction [1]. In this presentation a porous sample was prepared at 300 W rf power with He as process gas (at 4.96E-02 mbar) and an oblique angle deposition of 30^0.

The microstructure was investigated by transmission electron microscopy (TEM) techniques such as energy filtered TEM (EFTEM), and electron energy-loss spectroscopy (EELS). The latter also applied in scanning mode of the TEM (STEM) for high resolution analytical TEM. Studies were carried out in a FEI Tecnai F30 operated at 300 kV and equipped with a Gatan imaging filter (GIF) Quantum 963. STEM-EELS spectrum images were recorded with a pixel size of 1nm.

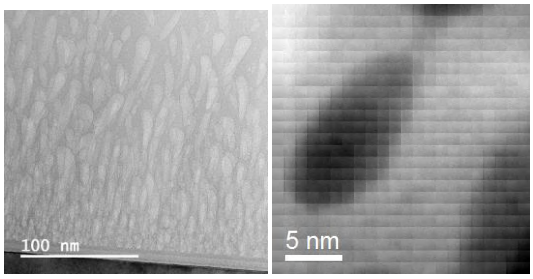

Fig 1. Left: TEM bright field image of porous silicon. Right: Spectrum-imaging HAADF signal showing one closed pore.

The closed pores aligned tilted ca. 30º from the substrate normal and show elongated shapes with typical pore diameter in the beam direction from 2 to 10 nm (see Figure 1). Tomographic reconstruction from TEM BF tilt series (±65°, 2° steps) also reveals the closed porosity with droplet like shapes.

As a main result it may be emphasized that by STEM-EELS (spectrum-imaging) we were able to detect Helium inside the pores, and also get a rough measure of the Helium pressure inside (2 to 0.2 GPa), well above the pressure of He in the deposition chamber (5 Pa). Our results are in agreement with reported data for Helium droplets trapped in solids as prepared by ion implantation. To our knowledge it is the first time that de quantification method here presented has been applied for detection and quantification of He gas in silicon with high lateral resolution.

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Effect of rare earth ion implantation on the structure of nitride semiconductors

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Recently, rare earths (REs) doped III-V nitride semiconductors (aluminum, gallium and indium nitrides) of wurtzite structure have received a particular attention due to their promising applications in optoelectronics. With their band gaps (AlN: 6.2 eV, GaN: 3.4 eV, InN: 0.7 eV), these materials have shown strong potentialities for the development of the next generation of multicolor devices, like full color displays or white LEDs. In this scope, ion implantation may be a desirable and easy way to introduce REs during the fabrication process of such devices. However, this technique also produces damage that need to be limited to avoid strong degradations of the material properties.

To this end, a continuous research effort has been going on to determine the behavior of nitride semiconductors submitted to REs implantation at room temperature and medium energy (300 keV) in the [10^{12} - 10^{17}] at./cm^2 fluence range. The main results that will be presented here evidenced significant differences in the damage build-up of InN, GaN and AlN. In the case of InN, transmission electron microscopy (TEM) points out a high sensitivity to ion beam damage and a fast surface decomposition at the lowest fluences (around 10^{12} at./cm^2) [1]. Despite structural similarities with InN, GaN and AlN exhibit stronger resistance to the implantation damage. By combining TEM with Rutherford backscattering spectroscopy / channeled and X-ray diffraction, we observe that the damage mechanisms are quite similar in these two materials, while the strain built-up and the final microstructure differ. In particular, it is shown that crystal defects, and especially stacking faults, play a critical role that leads either to a surface nanocrystallization of GaN ($2x10^{15}$ at/cm^2) or to a bulk amorphization in AlN at much higher fluences (> 10^{17} at/cm^2) [2]. The mechanisms involving the defects formation and their extension will be discussed to explain the different behaviors observed within this group of nitride semiconductors.

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Silver nanocubes as optical antennas for second harmonic generation in $RbTiOPO_4$ ferroelectric crystals

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Nowadays, there is an intense activity directed towards the fabrication and characterization of different types of plasmonic nanostructures since they can improve the performances of the existing optical and optoelectronic devices. Recently, it has been demonstrated that the polar surfaces of ferroelectric crystals offer a useful platform for polarization mediated chemistry, enabling a low-cost option for deposition of metallic nanostructures [1]. Additionally, ferroelectric crystals play an important role in photonics due to their suitable electro-optic and nonlinear properties for light control.

Here we focus our attention on $RbTiOPO_4$ (RTP) crystal, which offers some advantages over the extensively used $LiNbO_3$, as it is a higher optical damage threshold and a lower coercive field, which lead to the possibility of poling thick samples [2].

We report for the first time the fabrication of alternate ferroelectric domain structures in RTP by direct electron beam writing using a scanning electron microscope driven by a nanolithography software.

Taking advantage of these alternate polarity surfaces, and by means of a photochemical reduction method, metallic Ag nanocubes were selectively self-assembled on the positive domain surfaces of a periodically poled ferroelectric $RbTiOPO_4$ crystal used as template. The average size of the obtained nanocubes was 50 nm and their size dispersion was 15%.

The effect of the Ag nanocubes on the optical properties of the ferroelectric crystal is studied by analyzing the changes on the second harmonic generated (SHG) response of the ferroelectric crystal, which is mainly produced at the domain boundaries. The excitation of Ag nanocubes- localized surface plasmon modes, resonant with the quadratic nonlinear optical signal from RTP, produces an enhancement of the SHG, which depends on the surface coverage by Ag nanocubes. The results are of interest for the development of new photonic systems with enhanced nonlinear optical response at the nanoscale.

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A Donor Molecule in Silicon

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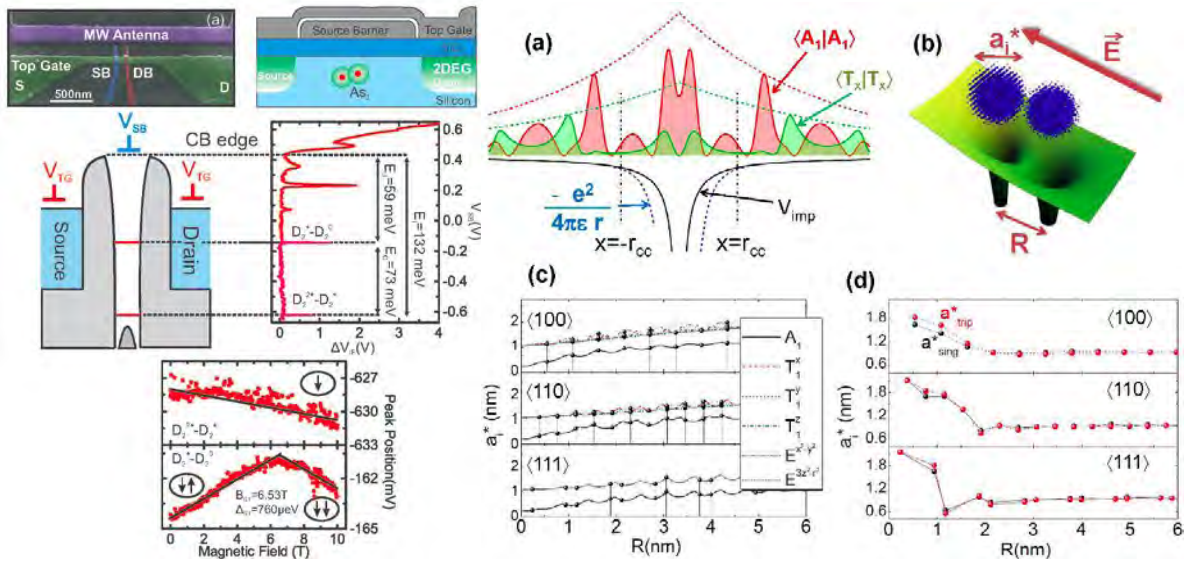
Substitutional donors in Si constitute analogues of atoms with giant electronic orbitals, extending over many Si neighbors around the donor. Its extent is large enough to integrate a single atom to electronic circuitry. Donor "molecules" of a few giant atoms open a potentially fruitful path towards scalable quantum devices. However, the analogy with traditional quantum chemistry only takes us so far, and a detailed understanding of the electronic structure of these molecular systems is a challenge yet to be overcome. By measuring the spectrum of a low-doped sample, we identify here a strongly interacting donor pair. The pair geometry is inferred by comparison of the measured spectrum with the one calculated in an effective mass theory incorporating the Bloch states multiplicity in Si, a central cell corrected donor potential and full configuration interaction. Finally, we theoretically ascribe the conditions for optimal performance of scalable donor based quantum electronics.



Raman scattering in single Bi_2Te_3 nanowires: Effect of the nanowire diameter and anharmonicity.

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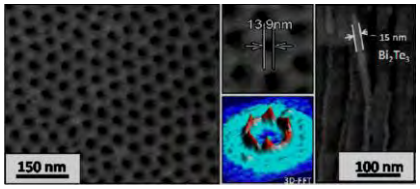

Fig. 1 Bi_2Te_3 15 nm NW arrays.

Bismuth telluride nanowire (NW) arrays of small diameters have being prepared. Porous alumina templates with porous sizes of 200, 40, 25 and 15 nm in diameter and 60 □m in length have being synthetized followed by the electro-deposition of Bi_2Te_3. Figure 1 shows an image of the template, a detail on a small region depicting the real size of the pores and the NWs obtained after removing the alumina in the template of smaller size. Small diameter Bi_2Te_3 NWs are strong candidates for the development of high efficiency thermoelectric modules.[1]

Bismuth telluride is a layered binary compound crystallizing in the $R\bar{3}m$ space group. It has 15 phonon modes. Since the space group is centrosymmetric, the 12 optical phonons are either "gerade" or "ungerade" (even and odd symmetry), depending on the lack of inversion symmetry in the vibration. There are 6 Raman active modes (the other six are infrared active), two E_g modes (bidimensional) and two A_g modes (one-dimensional). The four modes can be observed in most of the samples.

In this work, we analyze carefully the Raman selection rules of Bi_2Te_3 after a group theoretical analysis and label properly the optical modes appearing in the Raman spectra. We have studied the effect of quantum-confinement, anharmonicity and stress on the Raman modes of Bi_2Te_3. A profile analysis of the Raman peaks of the different NWs measured at high and low temperatures allows the separation of the effect of stress and anharmonicity. Concerning quantum confinement effects, they are expected only in very thin NWs, with diameters smaller than 15 nm.[2]

Based on the rigid ion model, we have calculated the phonon anharmonicities as a function of temperature. Although the model has been developed for bulk Bi_2Te_3, the effect of the surface has been taken into account into the calculations of the anharmonicity and stress.

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Raman measurements on thin-film nitride semiconductor compounds for photovoltaic applications

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The use of III-V semiconductor nitrides in solar cells has been of interest for the photovoltaics (PVs) community, due to the wide variation of the band gap in these materials [1].

Thin-film PVs based on crystalline, polycrystalline (with grain size at the micro or nano scale) and amorphous Si grown on Si or non Si-substrates have matured along the three last decades due to the advances in the design and processing of high-quality materials, solar cells and module assembling. Despite these advances, many fundamental and technological issues of great importance in order to achieve a further progress remain unsolved, including the further increase of the conversion efficiencies and the reduction of cost in thin silicon film-based solar cells.

On the other hand, tandem solar cells based on GaAs [2], [3] have shown to reach a very high efficiency, more than 40%, but the high production cost limits the use to space applications. The use of alternative materials, in particular the combination of wide and narrow gap nitride semiconductors, open a new challenge in the further improvement of high efficient solar cell for terrestrial applications in competition with silicon-based solar cells. Nitride semiconductors are particularly interested in this purpose because alloying only InN and GaN we can cover a wide spectral range, from the ultraviolet to the near infrared.

In this work, we analyze the quality of several nitride films for their use as PVs materials. Cubic GaN thin films have been grown by molecular beam epitaxy (MBE) on GaAs. The AlN and InN thin films have been grown also by MBE, but on Si (111) substrates. All the films were characterized by x-ray diffraction and Raman spectroscopy in order to investigate the crystal quality, homogeneity and stress in order to check its suitability as PV materials.

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Ab initio calculations of the stable and metastable crystal phases of MgSe

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We present a well converged *ab initio* study of the ground state structural and electronic properties of MgSe crystalizing in the rock salt, zinc blende, wurtzite and nickel arsenide phases [1] by using the full potential linearized augmented plane wave method as implemented in the Wien2k code. Our results for the total energy calculations indicates that the wurtzite structure is the most stable phase for MgSe at ambient pressure and that the rock salt and nickel arsenide are the high pressure phases of MgSe. From the calculated band structure, we found that the rock salt phase is characterized by an indirect band gap along $\Gamma - X$ and also NiAs phase is characterized by an indirect band gap along $\Gamma - K$ point while all the other phases are characterized by a direct band gap at the Γ −point. From the calculated total and partial density of states, we noticed that the main contribution to the lower valence band, comes from anion-s states ($Se - 4s$) as it is known for the II − VI compounds, however we found also that there are small contributions from $Mg - 3s$ and $Mg - 2p$ states at this energy while the upper valence band is dominated by $Se - 4p$ states and also there are contributions from $Mg - 3s$ and $Mg - 2p$ states then the lower conduction band is formed by mixing the $Mg - 3s$, and $Mg - 2p$ with $Se - 4p$, $Se - 4s$ and from $Se - 3d$ states.

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Growth and optical characterization of extremely long GaN Nanowires

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In the last years, there have been a number of studies done on gallium nitride (GaN) because of its promising electronic and thermal properties. Nowadays, GaN and related materials can be found in a number of commercial applications, such as solid-state lighting, ultraviolet lasers and are being investigated for high efficiency photovoltaics.

Moreover, GaN-based materials have potential application in monolithic solar-thermoelectric energy modules. Engineering band gap of materials by doping and alloying are effective approaches to reduce the high thermal conductivity and increase the electrical conductivity. The wide bandgap is one of the most characteristic features of GaN. It has been also demonstrated to have superior electrical performance and chemical stability at high temperatures.

In this paper we show the growth of long GaN nanowires, of several μm in length and characterize them by scanning electron microscopy, transmission electron microscopy, and photoluminescence and Raman techniques. The thermal conductivity of the nanowires has also been measured as a function of the diameter.