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OI-01

X-Ray microscopes at ALBA: TXM and XPEEM

Lucía Aballe

ALBA Synchrotron Light Facility, 08290 Cerdanyola del Vallès, Barcelona (Spain)

The ALBA Synchrotron Light Facility (Barcelona) is based on a 3 GeV, low-emittance storage ring which will feed an intense photon beam to a number of beamlines dedicated to basic and applied research.

Among the first phase beamlines, which will open to external users in 2012, there are two experimental stations dedicated to soft x-ray based microscopies: the Transmission X-ray Microscope (TXM) and the X-ray PhotoEmission Electron Microscope (XPEEM).

The TXM is installed at the bending magnet MISTRAL beamline and is a full-field microscope for imaging the transmission of samples of up to 10 micron diameter with a resolution of 30nm. It will allow imaging full hydrated cells and performing cryo-tomography in order to extract their three-dimensional structure.

The XPEEM is fed by the variable polarization CIRCE undulator beamline, and permits imaging surfaces with chemical, structural, and magnetic sensitivity down to a lateral spatial resolution of 30 nm. XPEEM has applications in a wide variety of fields such as surfaces and interfaces, nanostructures, or micro-magnetism. Contrast mechanisms based on x-ray absorption as well as on photoemission are available, thanks to an imaging electron energy analyzer with resolution below 0.2eV.

An overview of the TXM and XPEEM stations as well as application examples will be presented.

OI-02

EELS and HAADF study of defects in SrTiO3-x:Ny single crystal. The origin of Field-induced bi-stable resistive switching at the Al/$SrTiO_3$:N interface

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We found that the formation of “stacking faults” and other defects in perovskite structure is necessary for the formation of a bi-stable resistivity switching in the development of Resistance Random Access Memory (ReRAM) [1]. So far, the process of electroformation in the resistance bi-stability was not clearly described, which makes the data interpretation challenging. By simultaneous two-point/four-point resistivity measurements and thermal emission measurements, we observed local heating of the Al/SrTiO3:N interface (300ºC) during the electroformation, when Ohmic-like Al/SrTiO3:N interface becomes rectified due to the local oxidation of the anode. After the formation, the second and so on sweeps of I-V induce ions and/or oxygen vacancies movement in the vicinity of the anode/cathode, which is facilitated by threshold voltages and accompanied by increase of temperature up to 250-270 ºC. With the reduction scaling of microelectronic devices, lattice defects in these materials become increasingly important. Therefore, it is extremely demanding the careful characterization of defects produced during the material preparation, in our case by ammonia plasma treatment. Several questions arise in this work such as the type of defect, how the lattice distortion is around the defect, the local change in composition, and where the N is inserted in the structure. High-resolution transmission electron microscopy (HRTEM) is the first essential step for research on lattice defects. But, the correlation between structure and chemical composition and the distinct composition changes around the defects can be better studied by Z-contrast image (HAADF-STEM) and mapped with sub-nanometer spatial resolution utilizing EELS. On the basis of collected Ti $L_{2,3}$, O and N K-line EELS spectra around defect zones and free defect zones, bonding and composition information will be correlated with the atomic structure of $SrTiO_{3-x}:N_y$.

OI-03

Semiconductor nanostructures grown on GaAs nanoholes for quantum optical information technologies.

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The spatial matching between an isolated semiconductor nanostructure and a nanophotonic or nanoelectronic device is a mandatory requirement of important quantum optical information technologies.[1] The recent development of molecular beam epitaxy growth methods that produce quantum nanostructures directly on GaAs nanoholes might solve the problem of random nucleation that plague other growth methods.[2 3]

In this talk, I will comment on the optical properties of individual quantum dots[4 5] and quantum dot molecules[6] grown by these methods introducing some of their applications to quantum light sources and quantum logic devices.

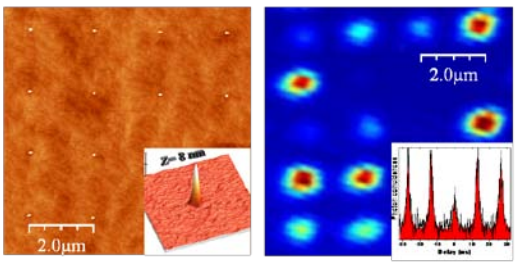

Fig 1. Ordered array of single photon emitters

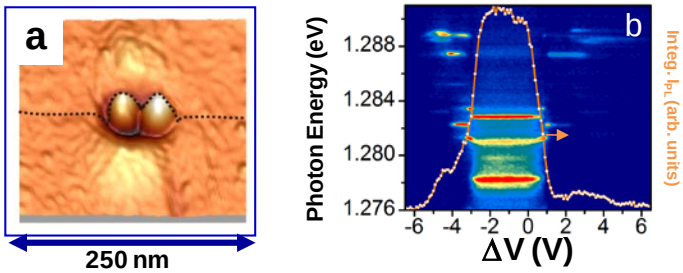

Fig 2 Single quantum dot molecule controlled by an external electric field.

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OI-04

"Multifunctional materials based on porous one dimensional photonic crystals"

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Porous one-dimensional photonic crystals (p-1DPC) are materials in which the refractive index varies periodically along one direction. These photonic structures have been identified as multifunctional materials due to the combination of their well connected porosity and their high optical quality of structural origin.[1] Our group developed two approaches to build these structures that are based on nanoparticulated films or on supramolecularly templated metal oxide layers. An overview of recent advances in the integration of different types of nanomaterials in these photonic crystals will be presented [2,3] as well as their capability to be infiltrated with liquids, vapors or polymers to develop applications in the field of sensing and in radiation protection.

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OI-05

Nanostructuring organic materials for plastic solar cells and photonic applications

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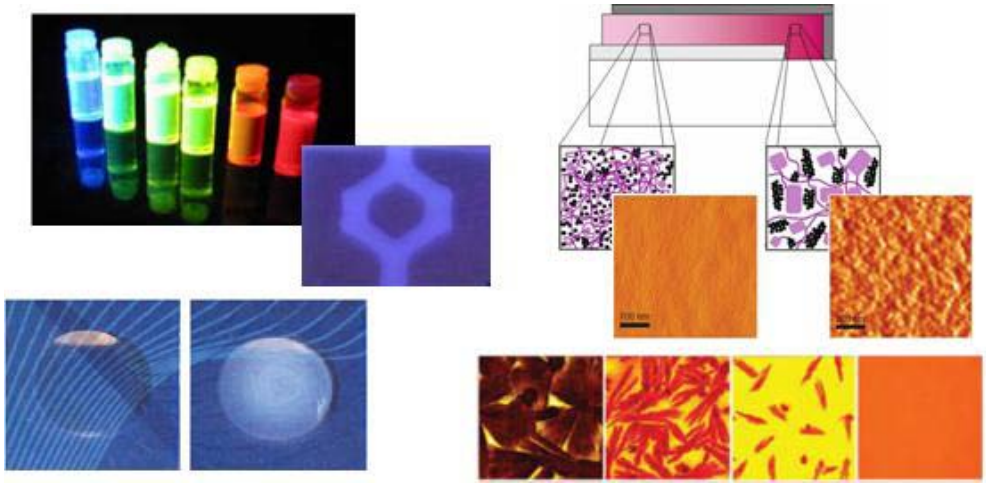
Why have polymers (*aka* plastics) become so prevalent in our world? Most people would answer that they are cheap structural materials, lightweight, easily manufactured into different shaped objects, and that they can be both relatively strong and brightly coloured. Now imagine the excitement that would ensue if one could combine the aforementioned traits of conventional polymers with other highly prized materials attributes: The controllable conduction and light emission/absorption/detection properties of traditional semiconductors that power the logic of computers, that underpin the digital revolution in entertainment (CD, DVD, etc), and that promise a means of efficiently harvesting solar energy.

These exciting novel materials, together with their applications, represent the focus of my talk. I will first introduce the main properties of organic semiconductors and then discuss some of our recent work on the interplay between nanomorphology and device performance. I will give examples of several optoelectronic devices made of organic semiconductors, including waveguides [1], dielectric mirrors [2], photodiodes [3] and solar cells [4] and discuss how controlling the spatially nanomorphology can open up the possibility of novel applications.



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OI-06

Generation and manipulation of pure spin currents

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Creation and control of spin currents is a key ingredient in spintronics, which has as a goal the use of the spin of the electron in addition to its charge. One way to create such spin currents is by using ferromagnetic (FM)/non-magnetic (NM) lateral spin valves. These powerful devices allow injection of a spin-polarized current from a FM injector into a NM channel by using a non-local geometry. With these, the spin current can be decoupled from the charge current and measured as a voltage using a second FM electrode [1]. Another approach to generate pure spin currents in nanostructured devices is using the Spin Hall effect [2], in which a charge current flowing along a NM material with strong spin-orbit coupling generates a transverse spin current. Alternately, spin currents can be generated without charge currents by applying a thermal gradient in a FM metal. In this fashion, spin currents are created by the recently discovered spin Seebeck effect [3].

For this reason, metallic lateral spin valves with transparent interfaces are fabricated by e-beam lithography and UHV evaporation [1]. We have studied the electrical spin injection and subsequent spin diffusion as a function of important experimental parameters such as injection current direction and magnitude, temperature, materials, and thickness.

We find that the spin injection is perfectly symmetric when applying low currents *from* the FM (spin injection) or *into* the FM (spin extraction), reversing exactly the polarity of the spin current in the NM [1]. This provides means for a pure electrical manipulation of the spin current polarity. In addition, thermal spin injection is observed at higher currents, arising from the spin Seebeck effect [3] in the FM.

We identify the effect of the surface and the interface on the spin diffusion length (λ) of the NM and the spin polarization (α) of the FM. The behavior of λ shows the different role of surface spin-flip scattering [4] in the various NM metals. In addition, the behavior of α for different FM metals helps understanding the contribution of the intrinsic polarization of the FM and the FM/NM interface in the spin injection efficiency. These experiments are relevant for the physics of spin currents and development of spintronic devices.

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OI-07

Spintronic nanodevices for energy-harvesting

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Spin related effects have been studied using electrical transport methods, by measuring the spin diffusing length in metals and semiconductors. In addition to electrical transport, the thermoelectric properties of magnetic materials are increasingly gathering more attention. There, magnons are believed to play an essential role. However, despite intensive studies on the spin transport, the coupling between electrons and magnons in ferromagnetic metals remains poorly known. We have studied the contribution of magnons to electrical and thermal transport in devices which consist of nano-sized permalloy wires with distinct coercive fields. At room temperature, we observe that the longitudinal magnetoresistance decreases linearly with magnetic field, because of a reduction of electron-magnon scattering processes due to magnon damping at high fields. We correlate these results with the Seebeck signal upon the application of a thermal gradient which gives the dependence of electron-magnon coupling with temperature. At low temperatures (T), the magnon drag effect is evident in the T3/2 power dependence of the measured signal. Whereas, above T=200K the magnon contribution is reduced because of magnon momentum loss from magnon-magnon scattering. These results demonstrate the feasibility of directly converting magnon dynamics of nanomagnets into an electrical signal and could pave the way to novel thermoelectric devices for energy harvesting [1].

The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement NANOFUNCTION n°257375.

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OI-08

Studying electron transport in single-molecule contacts

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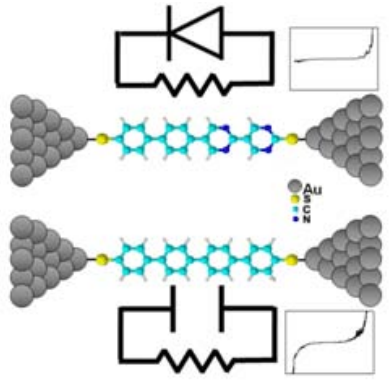
We describe our latest advances toward the fundamental understanding of charge transport in single-molecule electric contacts and how we can use this knowledge to tailor a desired electrical behavior in a single-molecule device. The first part will introduce the most common methods to characterize conductance on single-molecule contacts and we will describe new implemented methods to univocally identify when a single molecule contact is bridged between two macro-electrodes. The new methodologies are based on the introduction of fast AC mechanical perturbations along the electrode-electrode gap [1], as well as long pulling excursions applied as the final test to corroborate the single-molecule nature of the junction.



After the technical introduction, we will present few examples showing the feasibility of *tailoring charge transport behavior in single-molecule contacts through the molecular backbone design*. The first case presents one of the first examples of controlling diode (rectification) behavior in a single-molecule device [2]. We show that it is possible to go from a perfectly symmetric to a highly rectifying charge transport behavior in a single-molecule junction by introducing a specific asymmetry within the molecular backbone (see Figure 1), and how the surface preparation allows also control of the polarity of the final single-molecule diode. The second case shows an example of a single-molecule electromechanical actuator which uses a flat, poly-conjugated molecular moiety as the molecular component in the junction [3]. Here, the conductance can be modulated up to an order of magnitude by a mechanical control of the electrode-electrode separation. Finally, the last example deals with the design of new single-molecule field effect transistors (FET) by exploiting the previously introduced electrochemical gate method [4]. In this case, we will explore the use of graphene-like molecular scaffolds to achieve large conductance (high charge mobility) in our FET device. We demonstrate that the use of a bottom-up approach to build nanoscale single-molecule graphene junctions can provide with fairly high junction conductance and with a good ON-OFF ratio in the order of 1-100 [5].

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OI-09

New light on nano-materials under extreme compression: Synchrotron radiation and diamond-anvil cells

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The natural resonance between synchrotron light sources and high-pressure science has led to dramatic advances across surprisingly diverse scientific fields in previous decades. In particular, studies at high pressures are helpful for understanding the physical properties of the solid state, including such classes of materials as, metals, semiconductors, superconductors, among other [1]. Most progress in High-Pressure Research has been achieved thanks to the use of the diamond-anvil cell (DAC), a simple device capable of generating pressures almost as great as those found on the centre of the Earth [2]. With the DAC, by applying these pressures to micron-size samples, we can then study how materials behave under high pressures by a variety of analytical techniques. In special the combination of synchrotron radiation techniques (XRD, EXAFS, inelastic scattering, etc.) with the use of the DAC have had a profound effect on Solid State Physics and Chemistry. In recent years, this research extended from the study of bulk materials to nano-materials [3].
In this presentation I will review recent studied we performed on the structural, electronic, and lattice dynamics properties of different semiconductors and ceramic oxides. The reviewed results will include Raman and XRD measurements performed at room temperature up to 50 GPa. Differences and similarities between the physical properties of bulk and nano-materials will be commented. In particular, changes in compressibility and transition pressures will be discussed. Other questions like size effects, interaction between nanostructures and guest species or the interaction of the nano-system with the pressure-transmitting medium will be addressed. Finally, the possibilities opened by high pressure to nano-research will be discussed together with probable trends for the future research.

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OI-10

Silicon colloids: a platform for photonics, medicine and electronics

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Silicon colloids are micrometer size particles with a well defined spherical geometry and a very smooth surface. They are obtained by chemical vapour deposition means using di-silane as a precursor gas, and the type of silicon the colloids are made of can be amorphous, poly-crystalline or porous depending on the decomposition parameters.[1]

Silicon colloids are able to join three different technological areas, namely photonics, medicine and electronics, because they can sustain optical resonance modes,[2] they are biocompatible and an electronic circuitry can be build up on each particle since they are made of silicon. We will report about the progress achieved in these areas so far. Particularly, we will show how porous silicon colloids become a platform for a photonic encoding system[2] based on the photoluminescence properties of the particles, and we will report about their behaviour in biological environments.

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OI-11

Size-dependent electronic and magnetic properties of *single* iron-based nanoparticles probed by synchrotron x-ray spectromicroscopy

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Magnetic nanoparticles show a variety of unusual magnetic phenomenology when compared to the bulk materials, such as superparamagnetism, magnetic moment enhancement, and oddly shaped hysteresis loops [1]. In addition, there might be a breakdown of the usual scaling laws linking magnetic properties to size. These effects are due to the influence of the surface on magnetic interactions via bond breaking and charge rearrangement, and to the closeness of the particle size to critical magnetic length scales such as the domain wall width and the exchange length [2]. It is therefore essential to improve our understanding of the size-dependent evolution of the electronic states of the nanoparticles and of their hybridization at the interface with the supporting media, as well as of their spin configurations and particle-medium coupling mechanisms. This is difficult in ensemble measurements due to the role of interparticle interactions and also because essential effects of particular morphological parameters, preferential crystallographic orientations upon growth, or specific substrate defects may be averaged over.

In this work, we combine photoemission electron microscopy (PEEM) with synchrotron x-ray absorption spectroscopy (XAS) and magnetic circular dichroism (XMCD) to study element-specific electronic and magnetic structure of *individual* sub-30 nm iron metal [3,4] and iron oxide-based particles [5], at finite temperatures, supported on various substrates. For the Fe particles, size-dependent studies allow us to observe the transition from superparamagnetic fluctuations to stable ferromagnetic order at a particle size of about 12 nm. Single-particle magnetization curves in both the ferromagnetic and superparamagnetic states allow us to identify the role of the intrinsic magnetic anisotropy on the magnetic response. Further, we study $Fe_{3-x}O_4$ particles, synthesized by thermal decomposition, showing high crystalline quality and macroscopic bulk-like magnetic properties [5]. We observe that the local x-ray absorption spectra of single $Fe_{3-x}O_4$ nanoparticles cannot be fully superimposed to those of reference iron oxide species, suggesting that different iron oxide phases with competing electronic configurations and magnetic orders coexist inside the particle. This knowledge, which could not be obtained from average ensemble measurements, is essential to understand the collective behaviour of particles used in novel nanocomposite structures and bio-materials.

Finally, our approach opens new possibilities for a deeper understanding of the magnetization reversal in nanoparticles and their dynamical response to external stimuli.

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OI-12

Soft magnetic materials for energy efficient refrigeration

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The magnetocaloric effect, i.e. the reversible temperature change experienced by a magnetic material upon the application/removal of a magnetic field, is becoming a topic of increasing research interest due to the potential applications of this phenomenon for energy efficient and environmental friendly refrigeration at room temperature. From the materials science point of view, research on this topic is mainly focused on the discovery of new materials with low cost and enhanced performance (namely, magnetic entropy change, ΔS_M, refrigerant capacity, RC, and adiabatic temperature change, ΔT_{ad}).

While large ΔS_M and ΔT_{ad} peaks can be obtained in materials with a first order magnetic phase transition, this is at the expense, in most of the cases, of thermal and magnetic hysteresis. Moreover, acute peaks usually imply a smaller RC. At the same time, the magneto-structural phase transition which gives rise to the giant magnetocaloric effect requires large magnetic fields. These factors could limit the applicability of these materials for magnetic refrigeration and maintain the interest of studying those with a second order magnetic phase transition. In this talk we will overview the magnetocaloric response of soft magnetic amorphous alloys, which are low cost materials and can exhibit refrigerant capacities comparable or larger than GdSiGeFe [1], showing that these materials can play a role in this emerging field. It will also be shown that the use of these alloys as building blocks for developing biphasic layered composites can enhance the refrigerant capacity by ~90% with respect to the starting pure phases, if the appropriate selection of Curie temperature of the phases, value of the applied field and fraction of the constituents are selected [2].

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OI-13

Nonlinear optical effects in holey metal films

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Interaction of intense light with matter gives rise to great variety of nonlinear optical phenomena: Raman scattering, photo-luminescence in metals, Second Harmonic Generation (SHG), Four Wave Mixing (FWM), Third Harmonic Generation (THG) and Optical Kerr Effect (OKE) are among them [1]. The possibility of taking advantage from those or other nonlinear effects has attracted the attention of the scientific community, looking forward to getting active components at the nano-scale.

Steps towards the non-linear regime require better understanding on the behavior of non-linear materials at the nano-scale and, in particular when combined with nano-structured metals. In following that, we theoretically study OKE and THG in metal films pierced by periodically arranged slits [2]. We show the important role played by the metal properties and the particular geometry of the system in non-linear efficiency.

Finally we envisage the possibility of building an optical limiter of the transmitted intensity, in which the output intensity decreases when the incident one increases, and an optical switch, where the output intensity increases abruptly under a small change of the incident power [3]. These two operating modes are found in an array of metallic slits placed on a nonlinear Kerr-type dielectric layer, at the telecom regime. This approach relays on the abrupt changes of the output light intensity usually observed near linear transmission minima.

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OI-14

Electrostatic doping of high T_C superconductors

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The application of Field Effect Transistor (FET) concepts to electrostatically doped strongly correlated electron systems has been the focus of intense research during the last years [1] due to its potential impact on applied and basic science. From the technological point of view, the control of the charge carrier density by means of an applied electric field may provide a tool to modify the electronic and magnetic properties of novel materials in a reversible way. From a fundamental point of view, electrostatic doping would allow the systematic study of electronic correlations as a function of essential quantities such as electrostatic repulsion, hopping amplitude…, without altering the level of disorder associated with conventional chemical substitution.

In this talk we will show our recent results on Electronic Double Layer Transistor (EDLT) techniques applied to high T_C cuprates. The EDLT configuration, which employs ionic liquids as gate dielectrics, has succeeded in achieving unprecedented charge transfers, of the order of 10^{15} carriers/cm^2. This large accumulation and depletion of carriers allowed us to explore the phase diagram of $YBa_2Cu_3O_{7-X}$ and $La_2CuO_{4+\delta}$. We will focus on the physics of the superconductor to insulator transition [2] and discuss the magneto-transport properties of the underdoped and overdoped regions of the phase diagram [3].

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OI-15

Modelling electron transport at the nanoscale using plane waves

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In recent years, electron transport through nanostructures has attracted great interest, as nanoscale junctions or molecular devices may create a molecular electronics technology in the future. The current through a nanostructure, such as a single molecule, has been measured by means of scanning tunneling microscopy (STM) and breakjunction techniques. Because of the difficulty of experimentally investigating the influence of the detailed atomic structure on the electron transport through such a nanosystem, theoretical modelling plays a key role in the interpretation of experimental results.

In this talk, we report electron transport calculations obtained using our plane-wave based transport calculation method. Since the plane-wave basis set is considered to be variationally more complete than a localized basis set, numerically more accurate results can be expected from plane-wave calculations, specially in the description of the wave function in the vacuum region.[1] Hence, our quantum-transport-calculation method is expected to be well suited to describe transport properties both in tunneling and contact regime, and it could successfully reproduce transport properties in STM and breakjunction experimental scenarios. In order to illustrate this, we present transport simulations both in contact and tunneling regime.

For the contact regime case, we address the issue of molecular electronic switches, which have been recognized as strong candidates to succeed the silicon based technology. A molecular transistor based on torsion-angle conformation change driven by a gate electric field has been designed, and its transport properties have been studied using ab-initio calculations.[2]

With regard to tunneling regime transport, results on the simulation of field-emission resonances (FER) are presented. This class of resonances appear when the STM experiment is operated in the field-emission regime, i.e. at bias voltages larger than the tip work function. Since our method is suitable for large bias voltages and large tip-sample distances, and includes the effect of the tip in an ab-initio fashion, we believe it is a powerful tool for the study of FER.

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OI-16

Implementing strong correlations in a first principles transport code

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We implement strong correlations in the form of an Anderson impurity model in ab-initio transport calculations. The U term is added in one or several orbitals near the Fermi level and the second order self-energy is calculated following an interpolative scheme [1, 2] between the atomic limit (weak coupling) and the strong coupling limit. We apply this scheme to several molecules between metallic leads and show how the electronic and transport properties change as a function of the intraatomic electron-electron repulsion and the coupling strength. We also show how the evolution of the zero-bias conductance as a function of a gate voltage is affected by correlations and how temperature influences the transport properties.

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OI-17

Applications of aberration corrected STEM-EELS to transition metal oxides

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Transition metal oxides (TMO's) have been widely studied in recent years due to their impressive and yet far from understood properties. In these materials the oxygen atoms form strong covalent bonds with the partially filled *d*-states of the transition metal elements. These bonds play a critical role in determining the magnetic, thermodynamic, structural, elastic and electronic transport properties of TMO's. The ensuing physical properties are remarkably broad – insulating, semiconducting, metallic, superconducting, ferromagnetic and antiferromagnetic behavior, spin glasses, ferroelectricity, piezoelectricity, etc. Electron energy loss spectroscopy in the aberration corrected scanning transmission electron microscope (STEM) allows one to explore, simultaneously, the structure, the chemistry and the electronic properties of materials in real space and with atomic resolution. Combining these techniques, spatially-resolved measurements of quantities such as hole doping or spin state are possible. We will show that the degradation in magnetization and conductivity in $La_{0.5}Sr_{0.5}CoO_{3-\delta}$ (LSCO) very thin films can be understood [1] by mapping the changes of the complex O K edge pre peak . The O K edge is also sensitive to the spin state of Co atoms [2], and is used here to image a novel spin state superlattice in LSCO thin films in real space with atomic resolution [3]. Other examples to be described include $YBa_2Cu_3O_{7-\delta}$-$BaZrO_3$ nanocomposites, which have recently shown a remarkable improvement in critical current density and record pinning forces at high magnetic fields [4]. The functionality of these films is highly dependent on the morphology of the nanostructures and on the strain and local composition of the interfaces between the two component oxides.

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OI-18

Chemically derived graphene: electronic, structural and mechanical properties

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The promising electronic, mechanical and thermal properties of graphene for high demanding applications call for the need of approaches that provide access to large amounts of graphene monolayers.
Here we report on the electronic, mechanical and structural properties of single graphene sheets obtained via chemical reduction of graphite oxide, a promising route for the large scale production of graphene layers that offers the possibility to assemble them on insulating technological relevant substrates.
Chemically reduced single graphene oxide layers exhibit moderate conductivities due to the presence of defects remaining after reduction[1,2]. This moderate electrical performance can be extraordinarily improved by a CVD process to heal defects contained within the monolayers. In this manner, sheets with two orders of magnitude conductivity enhancement can be obtained[3], reaching mobilities that exceed those of the molecular semiconductors currently used in organic electronics.
From the mechanical point of view, AFM indentation experiments on suspended chemically derived layers reveal a Young modulus closely approaching that of pristine graphene[4].

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OI-19

The Kondo effect in molecular devices from first principles

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When a magnetic molecule is deposited on a metallic substrate or attached to metallic contacts its magnetic moment may actually be screened by the conduction electrons due to the Kondo effect. In view of possible applications of magnetic molecules for nanoscale spintronics and magnetic storage devices, it is important to reliably predict whether the Kondo effect will actually take place in a given system, and to understand if and how it can be controlled by various parameters such as the molecular conformation [1], ligands [2] and/or the type of substrate [3]. From a more fundamental point of view, magnetic molecules in contrast to most bulk systems offer the possibility to study exotic realizations of the Kondo effect such as the orbital Kondo effect [4] or the underscreened Kondo effect [5].

Here I present a *full ab initio* method for calculating the electronic structure and transport properties of molecular devices taking explicitly into account the strong correlations of localized electrons that give rise e.g. to the Kondo effect. My approach combines the COHSEX approximation with more sophisticated many-body techniques like the One-Crossing-Approximation and the Dynamical Mean-Field Theory for treating strongly interacting localized electrons properly. It is a further development of our previous method based on Density Functional Theory [6,7] that was not yet fully *ab initio* due to its dependence on the screened interaction between the localized electrons as a parameter. This screened interaction can now be calculated on a first principles basis within the COHSEX approximation.

The application of this new method to magnetic atoms and molecules attached to metallic leads or deposited on surfaces sheds light on the complex nature of the Kondo effect in molecular-scale devices.

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OI-20

Josephson current in carbon nanotubes with spin-orbit interaction

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We demonstrate that curvature-induced spin-orbit (SO) coupling induces a 0-□ transition in the Josephson current through a quantum dot carbon nanotube coupled to superconducting leads [1]. Our calculations, which cover all relevant transport regimes, non-interacting, Coulomb Blockade, co-tunneling and Kondo, determine in a precise manner the conditions for the transition in terms of system parameters, which can be tuned experimentally. Our predictions are relevant in view of recent experimental advances in transport through ultra-clean nanotubes with SO coupling.

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OI-21

Nanoenginering Thermoelectric for the 21st century applications

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One of the major social problems for the 21st century is going to be making available a sustainable supply of energy to the world's population since world demand increases while fossil fuel supplies decrease.
Thermoelectric energy converters are solid-state devices are able to convert waste heat into electricity, with no moving components, they are silent, totally scalable and extremely reliable. For all that reasons, they are expected to play an increasingly important role in meeting the energy challenge of the future.
Some of the most important advances in enhancing the efficiency of these materials are found in their nanostructuration. In this talk, a review of the state of the art in thermoelectric nanomaterials will be presented.

Phase-Field Models for Microstructural Studies

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Essentially, the phase-field method assumes that the free energy of a system may be written as a functional of conserved (i.e., phase-fields) and non-conserved (i.e. composition fields) continuous field variables. The evolution of such a system is then ruled by the Cahn-Hilliard non-linear diffusion equation and the Allen-Cahn relaxation equation. Since its emergence, the phase-field method has become a powerful computational tool to study the morphology and microstructural evolution in materials and simulate relatively complex processes including solidification, solid-state phase transformations, grain growth, crack propagation or dislocation microstructures, among others. This lecture states the fundamentals of the various models for phase-field and reviews some of its applications in Materials Science. A critical analysis of its successes and faults will follow.

OI-23

Tuning magnetic properties of out-of-plane and in-plane magnetic anisotropy media: from thin films to patterned nanostructures

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Properties of magnetic thin films differ from those of bulk materials due to the reduced dimension in thickness. Following this reduction of dimensions by patterning the thin films into magnetic elements with laterally constrained dimensions will yield novel spin configurations, caused by boundary conditions and geometric factors. Current lithography techniques allow the fabrication of magnetic structures with lateral sizes from few to hundreds of nanometers. The evolution of magnetic properties from thin film to patterned nanostructures is described for two magnetic systems, i) exchange coupled bilayers with in-plane magnetic anisotropy, and ii) thin films with out-of-plane magnetocrystalline anisotropy.

Exchange coupled antiferromagnetic (AF)/ ferromagnetic (FM) bilayers of FeF_2/Ni have been grown on a single crystal of MgF_2 (110) surface orientation. FeF_2 is AF below its Néel temperature, 78 K. Uncompensated spins yielding exchange bias (EB) are antiparallel coupled to the Ni magnetization, which leads to negative EB at low cooling field (H_{FC}) and the appearance of positive EB at high H_{FC}. The minimum H_{FC} necessary for positive EB can be tuned in patterned thin films. The smaller the size of the nanostructure the lower the H_{FC} giving positive EB. This result is explained taking into account the patterning effects on the AF domains that modify the balance between Zeeman and exchange energies [1].

Another interesting patterning effect has been observed in CoCrPt nanostructures with out-of-plane magnetocrystalline anisotropy. Unpatterned thin films of 10- and 20-nm thick CoCrPt exhibit out-of-plane anisotropy. However the net anisotropy of patterned lines and rings, with widths from 2 μm to 100 nm, evolves from out-of-plane to in-plane and transverse to the line axis, and finally to in-plane and parallel to the line axis as the width becomes smaller. This magnetic behavior is explained considering the magnetocrystalline, magnetoelastic, shape and surface energies of the patterned structures [2].

These two examples point out relevant consequences of lateral confinement that must be carefully considered in the design of spintronic devices and patterned magnetic storage media. Authors acknowledge funding from Spanish MICINN grant MAT2010-20798, SA-2010700053 and DFV/6/12/TK/2010/24

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OI-24

Interfacial physical phenomena in magnetoelectric systems

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The magnetic properties of epitaxial thin films can be controlled either thermally or electrically via strain from ferroelastic-ferroelectric substrates[1,2]. These strain-mediated magnetothermal and magnetoelectric effects, which promise valuable applications such as electric-write magnetic-read memory devices[3], depend dramatically on the film-substrate coupling across the interface and the interplay between magnetic and structural degrees of freedom on the film. Here, we report temperature- and electric-field-driven changes in the magnetization of $La_{0.7}Ca_{0.3}MnO_3$ and $La_{0.67}Sr_{0.33}MnO_3$ manganite films grown on traditional ferroelectric $BaTiO_3$ and relaxor ferroelectric $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ substrates. Using temperature as driving parameter, we achieved large and reversible magnetic entropy changes in $La_{0.7}Ca_{0.3}MnO_3$ films on $BaTiO_3$ substrates. These entropy changes can be isothermally driven by external magnetic field to yield extrinsic magnetocaloric effects comparable with the best magnetocaloric materials[4]. Using electric-field as driving parameter, we achieved large changes in the magnetization of $La_{0.67}Sr_{0.33}MnO_3$ films on $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ substrates, which depending on operating temperature are either sharp and persistent, or continuous and reversible. Macroscopic results (magnetometry) will be presented to demonstrate these magnetothermal and magnetoelectric effects, and microscopic results (photoemission electron microscopy with x-ray magnetic circular dichroism contrast and ferromagnetic resonance) will be presented for insight into the underlying physical mechanisms that permit this myriad of functional properties.

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OI-25

Functional mesoporous nanocast hybrid materials

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The synthesis of mesoporous materials by multi-step nanocasting is becoming increasingly appealing due to their novel properties and potential applications in a broad range of fields including gas-sensing, heterogeneous catalysis and magnetic hyperthermia therapy [1,2]. To date, many single transition metal oxides displaying large surface-to-volume ratios have been already prepared as negative replicas of ordered mesoporous silicas (e.g. SBA-15, KIT-6, SBA-16, MCM-41, etc). The nanocasting pathway has been recently extended to complex oxide systems such as double oxides and spinels in order to enhance the functionality of the mesoporous replicas. Hereby we present two different synthetic approaches based on the nanocasting pathway for the preparation of magnetically active ordered mesoporous metal oxides, using either SBA-15 or KIT-6 silicas as hard templates [3-5].

In the first approach, the SBA-15 silica template was impregnated with different proportions of nickel and cobalt nitrate salts followed by calcination at 550ºC. The SiO_2 template was finally etched away to release thermally stable $NiO/NiCo_2O_4/Co_3O_4$ composite replicas [5]. The magnetic properties, i.e., the saturation magnetization (M_S) and the coercivity (H_C), could be continuously varied given the ferrimagnetic (FiM) ($NiCo_2O_4$) and antiferromagnetic (AFM) (NiO and Co_3O_4) character of the constituents [5]. Interestingly, the $NiCo_2O_4$-rich composites were FiM at room temperature (Fig. 1), and could consequently be easily manipulated using small fields.

In the second one, highly ordered mesoporous AFM Co_3O_4 KIT-6 replicas were used as hosts to accommodate a FiM component within their gyroidal framework. For this purpose, the Co_3O_4 KIT-6 materials were impregnated with iron nitrate salt and subjected again to calcination. On calcining, the iron nitrate rendered a FiM spinel-type $Fe_xCo_{(3-x)}O_4$ layer on the surface of the pores. The magnetic properties showed that H_C of $Fe_xCo_{(3-x)}O_4$ was dramatically enhanced when the material was cooled below the Néel temperature (T_N) of the AFM Co_3O_4 host. Moreover, the system exhibited a loop shift in the field axis below T_N, which is characteristic of AFM-FiM coupling [6]. Significantly, H_C and H_E could be controlled by the cooling field.

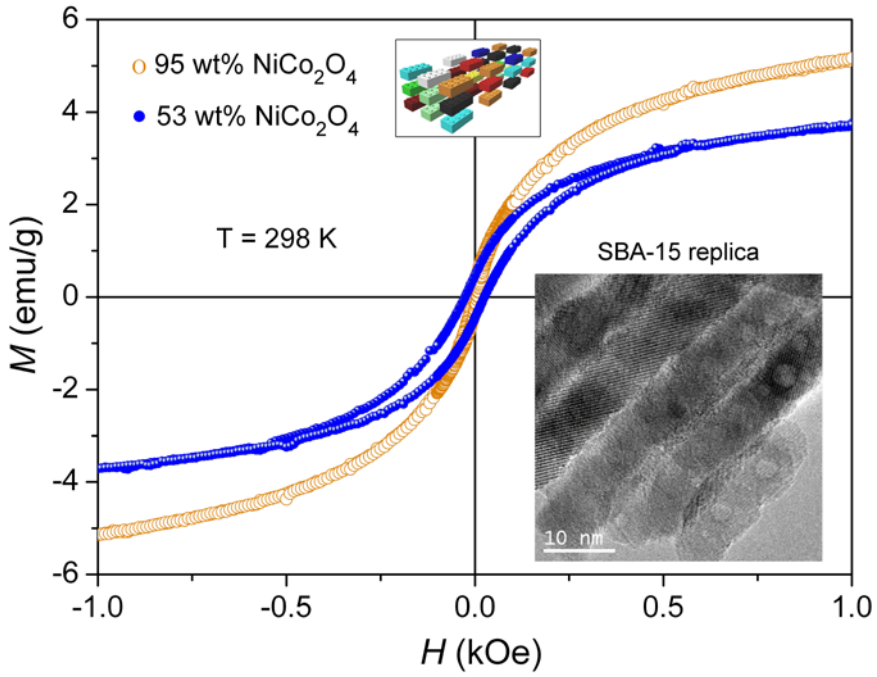

Figure 1. Room-temperature magnetic hysteresis loops of SBA-15 templated $NiO/NiCo_2O_4/Co_3O_4$ composites with different amounts of FiM $NiCo_2O_4$. The inset shows a high resolution transmission electron microscopy (TEM) image of the composites.

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OI-26

Anharmonic flexural phonons in graphene

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Graphene is a two-dimensional (2D) crystalline membrane of carbon atoms, which unusual properties have attracted an enormous interest. Graphene has been demonstrated to be stable even for free-standing samples. Crystalline membranes at finite temperatures have an anomalous behavior of the bending rigidity that makes them more rigid in the long-wavelength limit. This issue is particularly relevant for applications of graphene in nanoelectromechanical and microelectromechanical systems. We calculate numerically the height-height correlation function of crystalline two-dimensional membranes, determining the renormalized bending rigidity in the self-consistent screening approximation (SCSA). For parameters appropriate to graphene, the calculated correlation function agrees reasonably with the results of atomistic Monte Carlo simulations for this material.

Furthermore, in practice, physical membranes are exposed to a certain amount of external strain (tension or compression) due to the environment where they are placed. As a result, the behavior of the phonon modes of the membrane is modified. We show that anharmonic effects in stiff two-dimensional membranes are highly suppressed under the application of tension. For this, we consider the anharmonic coupling between bending and stretching modes in the SCSA and compare the obtained height-height correlation function to the corresponding harmonic propagator. The elasticity theory results are compared to atomistic Monte Carlo simulations for a graphene membrane under tension. We find that, while rather high values of strain are needed to avoid anharmonicity in soft membranes, strain fields less than 1% are enough to suppress all the anharmonic effects in stiff membranes, as graphene. Finally we will consider the effect on the resistivity of electron interaction with flexural phonons. We will discuss the temperature and doping dependence of this contribution, treating the out of plane vibrations beyond the harmonic approximation.

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OI-27

Electromechanical properties of catalyst grown Silicon Nanowires and their application for nanoelectromechanical devices

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The catalytic growth of semiconductor nanowires offers the possibility of achieving otherwise unfeasible structural conformations and material combinations at the nanoscale that result in unique physical properties [1]. In consequence, nanowire devices based upon such bottom-up nanofabrication approach, in which functional quasi-1D nanostructures are assembled from chemically synthesized building blocks, have the potential to go beyond not only the size reduction limits, but also the device functionality constraints of top-down lithography based technologies. This is particularly significant for nanoelectromechanical systems (NEMS) because their basic properties are greatly influenced by scaling-laws, thus resulting in completely extreme or different behaviour at the nanoscale. Silicon nanowires obtained via the vapour-liquid-solid (VLS) mechanism offer exceptional perspectives for applications in NEMS. Their structural quality (low defect density, low surface roughness) and unique electromechanical properties (high stiffness and resonance frequencies, giant piezoresistance) together with recent advances in growth control, promise to allow unprecedented performance of NEMS.

In this presentation we will describe several results concerning the fabrication, characterization and performance optimization of several Si NW based NEMS devices. By combination with top-down micro/nano fabrication methods, the VLS synthesis can be used to produce horizontally suspended nanowire beams doubly clamped between the sidewalls of prefabricated Si microstructures [2]. This approach can be applied to obtain single nanowire or nanowire array based beam-like structures [3], which serve as basic building blocks for nanomechanical devices. The characterization of the elasticity [2], piezoresistance [4] and mechanical resonances [5] of such structures has lead us to propose the development of nanomechanical resonators and piezoresistive transducers as devices that would directly benefit from the nanowires properties. It will be discussed how nanomechanical resonators based on individual, extremely small nanowires can provide a detection limit for inertial mass sensing close to that required for atom resolution mass spectrometry, whereas piezoresistive strain gauges based on highly dense nanowire arrays can be applied to obtain cantilevers with a detection limit for displacement sensing up to ten times better than that provided by conventional Si thin film piezoresistive cantilevers.

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OI-28

Localization in twisted graphene bilayers

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We study the problem of charge localization and zero-mode formation in twisted and sheared graphene bilayers. Such systems exhibit a periodic Moiré pattern in the interlayer coupling due to the mismatch between layers. We show that charge localization, recently observed in by STM measurements [1], may be explained without the need of electron-electron interaction, as the effect of an effective non-Abelian gauge field that emerges naturally from the spatial modulation of the interlayer hopping. Additionally, we demonstrate the recurrent vanishing of the Fermi velocity (zero mode formation), numerically predicted to occur at certain discrete values of the the Moiré pattern period [2], and explain it in terms of the non-Abelian effective potential. Our results suggest the possibility of exploring two-dimensional non-Abelian gauge physics in a controllable solid state setting.

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OI-29

First-principles nanoelectronics: Oxide thin-film devices by design

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Complex oxides are characterized by a multitude of coupled electronic and lattice degrees of freedom, and therefore constitute an unusually rich playground for experimentalists and theoreticians alike. These microscopic variables manifest themselves in macroscopically measurable quantities such as polarization, magnetization and strain, whose mutual co
upling is sought after for applications in multifunctional electronic devices.

To understand the interplay of these many factors, density functional theory (DFT) has proven an i
nvaluable tool. However, the treatment of the macroscopic electrical variables (electric fields and polarization), which are a crucial ingredient in describing the experimentall
y observed response properties, has traditionally been difficult within first-principles calculations. In this talk I will review a number of recent methodological develop
ments that removed this limitation, thus extending the scopes of first-principles theory to the simulation of realistic devices within arbitrary electrical boundary conditions [1,2].

Moving to the applications, I will first discuss the evolution of the band offset at a metal/ferroelectric interface as a function of polarization [3], and its implications for the electrical properties of nanocapacitors. Next, I will show that, depending on the polarization of the film, a problematic regime might occur where the metallic carriers populate the energy bands of the
insulator, making it metallic. [4] As the most common approximations of density functional theory are affected by a systematic underestimation of the fundamental band gap of insulat
ors, this scenario is likely to be an artifact of the simulation. I will discuss a number of criteria to systematically identify this situation in simulations, and effective mod
eling strategies to describe this peculiar charge compensation mechanism.
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OI-30

Quantitative Soft X-Ray Resonant Reflectance Spectroscopy of thin oxide films

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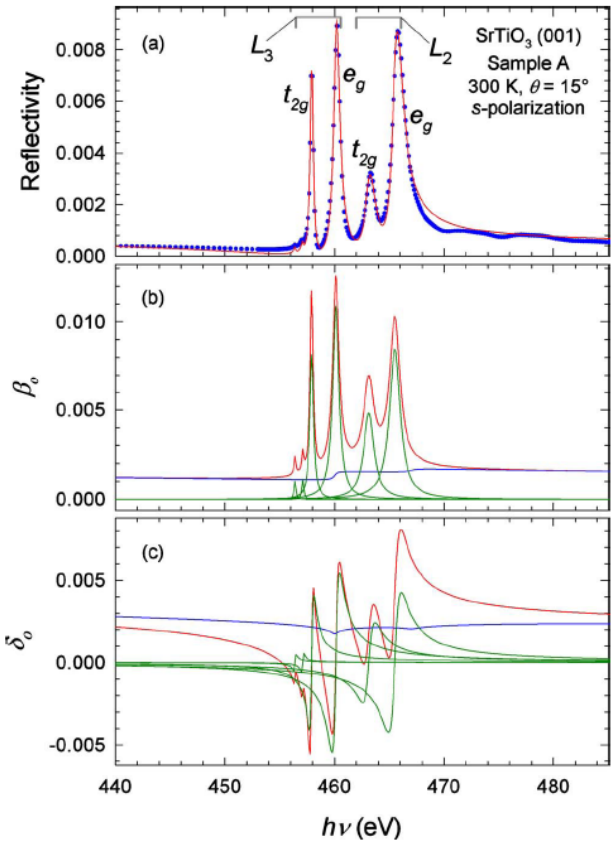
A quantitative approach for x-ray resonant reflection spectroscopy has been recently proposed and applied to the analysis of reflectance spectra R(hν) measured in SrTiO3 (001) single crystals across the Ti L2,3 soft x-ray edges[1]. This approach allows to sense the near-surface region differently than other techniques such as resonant XAS via total electron yield, which at a price of a fitting analysis step provides extended spectroscopic information.

Modeling the reflectivity measured at x-ray fixed incident-angle but varying photon energy, R(hν), provides absolute resonant optical properties $n = 1 - \delta - i\beta$ indicating short skin depths (< 10 nm) when tuned to the $t2_g$ and e_g peaks.



Resonant R(q) exhibits clear structure revealing a subsurface layer several nm thick having different properties from the bulk, which could be at the origin of observed and a priori unexpected room temperature linear dichroism. These results will be discussed in the context of established and recent studies of the STO surface and their relevance to dielectric and ferroelectric properties of STO surfaces and thin films.

Further development of this general methodology via a variational approach as well as its application to other systems will be briefly presented[2,3].

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OI-31

"Superconducting qubits: from quantum optics to condensed matter physics on a chip"

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Cavity QED or the art of controlling the light matter interaction has applications in lasing, nonlinear optics or quantum information processing to say some. Besides, cavities and atoms allow for beautiful and fundamental experiments. Some years ago solid state physics began to imitate the optical layouts. Depending on the implementation cavities were replaced by photonic crystals, transmission lines, atom ensembles or nanoresonators, while atoms where mainly replaced by their artificial counterparts as quantum dots or superconducting qubits.

The field of cavity QED on the solid state has attract interest of many labs making its progress quite impressive in the last years. After the first seminal experiments showing the strong coupling regime between (artificial) atom and cavity new ideas and experiments appear: Wigner reconstruction, coupled cavity architectures, quantum-classical limits, etc… Further, the possibility of these systems to reach the so called ultra strong coupling limit has been also demonstrated. In this limit the light-matter coupling is of the same order than the atom/cavity transition frequency. As a consequence the usual first order exchange transitions between the atom and cavity are not sufficient and non perturbative transitions emerge.

In this talk I will overview the different regimes of light matter regimes in solid state devices. I will discuss several architectures in which we are working, and I will motivate this research by proposing them as good candidates for studying many body physics, such as quantum phase transitions.