

# JPhD2017

## 3rd Scientific Meeting of BNC-b Students



**Oral Presentations**

## Thermoelectric properties of 2D materials and thermoelectric properties of topological Insulators

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The main idea is to study the thermal conductivity of 2D materials with the help of the Raman thermometer - a contactless technique. In order to do so, one of the challenges was to manage to transfer suspended flakes of 2D materials. The utilization of a dry transfer method has been used to transfer on some holes. MoS<sub>2</sub> flakes have been exfoliated and suspended structures have been made.

In the other part of the study about thermoelectric devices with topological insulators, we studied the Dirac states of TIs in the case of thermoelectric properties. This can lead to improve the power factor. Different alloys of (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> have been grown by MBE on a (111) Barium Fluoride substrate. Usual XPS measurements were made in order to see the different concentration. In addition, ARPES and Hall measurements combined to define the surface states. Finally, thermoelectric devices were designed by lithography in the objective to measure the Seebeck coefficient.

# Plasmonic response of a triangular array of nanogaps: high absorption and extended temporal response

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Plasmonic nanoparticle arrays have been widely used for a variety of applications including enhanced spectroscopies, perfect absorbers, plasmonic lasing or energy harvesting. Uncountable research has been done in the characterization of individual antennas as well as arrays in which the nanostructures interact via near-field or far field coupling. In particular, arrays with honeycomb lattice have been studied and theoretical results proved that these arrays present collective plasmon modes similar to those of graphene.<sup>1</sup> However no experimental results have showed any outstanding effect related to the mentioned lattice.

We have investigated plasmonic arrays of metallic nanostructures consisting of triangular lattices of asterisk-shaped gold nano-elements of 300 to 500 nm separated by gaps ranging from 20 to 100 nm. A metal-insulator-metal (MIM) configuration, in particular Au-SiO<sub>2</sub>-Au, has been used to optimize the system response.<sup>2</sup> Their electromagnetic response has been simulated using Finite Difference Time Domain (FDTD) simulations showing two interesting features: first, a narrow peak in the visible region of the spectrum corresponding to an almost complete absorption, and second, the fluctuation of the system between two geometrical configurations of the excitation modes that lingers for a remarkably longer time than the excitation pulse length.

A set of samples has been fabricated by electron beam lithography (EBL) on glass substrates and with a MIM configuration. By using EBL as the lithography method, the resonances can be easily engineered to match the desired wavelength. These structures could therefore be of interest for SERS or for applications based on light absorption such as photovoltaics.

## Acknowledgements

This work was supported by Spanish MINECO (MAT2015-68772- P), Catalan DURSI (2014SGR220), and European Union FEDER funds (Una manera de hacer Europa). A. Conde-Rubio acknowledges Spanish MINECO for a Ph.D. contract (BES-2013-065377).

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## **Nanoscale characterization of electronic devices based on novel materials**

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The transistors, the basic building blocks of the integrated circuits (IC), now have sizes of only several nanometers following the scaling predicted by the Moore's law. Due its small sizes, several problems and faults arise that need to be addressed. Other materials have been proposed to substitute the traditional SiO<sub>2</sub> to solve these scaling problems, for example, high-k dielectrics and since the emergence of graphene, 2D materials but is necessary a profound study of such materials to understand its influence in such small devices. As tiny variations of properties in the material could have a huge impact on the nanodevice, the objective is to perform measurements of nanoscale properties of new materials using Atomic Force Microscopy (AFM) related techniques, like conductive-AFM or Kelvin Probe Force Microscopy (KPFM). In this work, the analysis of a thin TiO<sub>2</sub> gate dielectric and a graphene based channel is presented. In particular, the TiO<sub>2</sub> have been analyzed for the development of FinFET and nanowire transistors simulations. On the other hand, devices with oxidized graphene the active material have been obtained and studied at device and nanoscale level.

## Initial stages of mixed nickel-iron oxides growth on Ru(0001)

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Transition metal oxides (TMO) are promising candidate materials for future spintronic devices. Their properties arise from the interaction between transition metal and oxygen ions in a given structure which are very sensitive to different bond length and angles, as well as to their particular cationic distribution. Among them, the spinel family comprises a large number of compounds. Spinel has an fcc anion lattice with cations occupying tetrahedral and octahedral sites. Spinel can be half-metallic (like  $\text{Fe}_3\text{O}_4$ ), ferrimagnetic insulators, superconductors ( $\text{LiTi}_2\text{O}_4$ ) or heavy fermion materials. However, their properties in thin film growth, as necessary for devices, are often disappointing, dictated by the defect density. Here we demonstrate a method for preparing high quality ultrathin TMO films on a metallic substrate. Mixed nickel-iron oxides have been grown on Ru(0001) by oxygen-assisted molecular beam epitaxy at elevated temperatures (800 - 900K). The nucleation and growth process are observed in situ by means of Low Energy Electron Microscopy (LEEM). A comprehensive characterization is performed combining LEEM for structural characterization and PEEM (PhotoEmission Electron Microscopy) with synchrotron radiation for chemical and magnetic analysis via X-ray Absorption Spectroscopy and X-ray Magnetic Circular Dichroism (XAS-PEEM and XMCD-PEEM, respectively). The latter permits imaging the element specific magnetic domain structure.

The combination of in-situ experiments and micromagnetic characterization allowed us to determine magnetic domain configuration at microscopic level.

## **Strong anisotropy spin relaxation in graphene/transition metal dichalcogenide heterostructures at room temperature**

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Graphene has emerged as the foremost material for future two-dimensional spintronics due to its tuneable electronic properties. In graphene, spin information can be transported over long distances and, in principle, be manipulated by using magnetic correlations or large spin-orbit coupling (SOC) induced by proximity effects. In particular, a dramatic SOC enhancement has been predicted when interfacing graphene with a semiconducting transition metal dichalcogenide, such as tungsten disulphide ( $WS_2$ ). Here, we unambiguously demonstrate anisotropic spin dynamics in heterostructures comprising graphene and  $WS_2$ . We observe that the spin lifetime varies over an order of magnitude depending on the spin orientation, indicating that the strong spin-valley coupling in  $WS_2$  is imprinted in the graphene and felt by the propagating spins. Combined with spatial relaxation, the anisotropy can be used to fabricate a filter that modulates the transmission of spins depending on their orientation.

## **Multifunctional cellulose based photonic architectures**

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Cellulose is the most abundant polymer on Earth and for centuries has had a wide technological impact in areas such as textile, packaging or knowledge storage. It is biodegradable, biocompatible and possesses excellent mechanical characteristics that have raised the interest of many engineering fields. The versatility of cellulose has opened new venues in advanced materials in electronics, energy or biological applications. Here we introduce a cellulose derivative as an eco-friendly and water developable resist. We combine cellulose with nanoimprinting lithography (NIL), the most promising method for mass-produced inexpensive nanostructures over large areas and with a very low density of defects. Using cellulose as a resist and NIL, we are able to pattern silicon wafers or fabricate metallic nanoparticle arrays using water as the only solvent. Furthermore, we revolutionize the field of transient photonics by directly molding the cellulose itself into photonic and plasmonic architectures and illustrate their outstanding performance in several applications such as structural colour, photoluminescence enhancement and as disposable Surface Enhanced Raman Scattering substrates.

## Three-dimensional photonic crystals self-assembled from polyhedral metal-organic framework particles

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Self-assembly of particles into long-range, three-dimensional, ordered superstructures is crucial for the design of a variety of materials, including plasmonic sensing materials, energy or gas storage systems, catalysts and photonic crystals. Here, we have combined experimental and simulation data to show that truncated rhombic dodecahedral particles of the metal–organic framework (MOF) ZIF-8 can self-assemble into millimetre-sized superstructures with an underlying three-dimensional rhombohedral lattice that behave as photonic crystals. Those superstructures feature a photonic bandgap that can be tuned by controlling the size of the ZIF-8 particles and is also responsive to the adsorption of guest substances in the micropores of the ZIF-8 particles. In addition, superstructures with different lattices can also be assembled by tuning the truncation of ZIF-8 particles, or by using octahedral UiO-66 MOF particles instead. These well-ordered, sub-micrometre-sized superstructures might ultimately facilitate the design of three-dimensional photonic materials for applications in sensing.

## Gold nanoparticles arrays as tunable plasmonic crystals for SERS

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Gold nanoparticles (AuNPs) represent an effective platform for surface-enhanced Raman spectroscopy (SERS). The assembly of AuNPs into larger architectures further adds functionality and tunability to the optical properties exhibited by the individual colloids. Controlling the optical properties by the organization of AuNPs into supercrystals, thus, facilitates the use of NIR excitation wavelengths, which are optimal for the probing of biological media. However, despite the development of advanced colloid synthetic routes leading to high quality and practically monodisperse nanoparticles the fabrication of hierarchically structured materials based on plasmonic particles actuating in the visible and near infrared range remains a challenging task.

In this talk we present a straightforward method to produce large area plasmonic crystals with sub-micrometre periodicity using prepatterned soft molds. We demonstrate the assembly of AuNPs into hexagonal and square lattices with pitch sizes as low as 400 nm. Optical characterization of the supercrystals by means of vis-NIR microspectroscopy allows the identification of distinct plasmonic resonances that can be attributed to the periodic arrangement of the metallic clusters. Further, we show the tunability of the Bragg-SPP resonance throughout the visible and into the NIR range. Consequently, our supercrystals can be designed to act as SERS substrates that are specifically tailored for the desired excitation wavelength most suitable for the analyte under investigation.

# Nanoscale characterization coupled to multi-parametric modelling of High Five cells transient transfection

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High Five cells are one of the preferred platforms towards the production of recombinant proteins with the Baculovirus Expression Vector System (BEVS). Although it is a powerful system, the use of BEVS entails several limitations inherently associated to the viral nature of the infection. Growing interest has emerged on exploiting the potency of this host devoid of BEVS usage. Despite of numerous efforts involving the use of polyethylenimine (PEI)-based reagents or expensive transfection carriers, there is not an efficient and scalable protocol for these cells yet. Here, a PEI-based transient transfection method has been developed for suspension adapted High Five cells in Erlenmeyer flasks. Method optimization was performed with the model proteins intracellular enhanced Green Fluorescent Protein (eGFP) and Secreted Alkalyne Phosphatase (SEAP).

Nanoscale characterization was performed to select NaCl 150mM as the DNA:PEI complexation solution. Cryo-Electron Microscopy (Cryo-EM) and Dynamic Light Scattering (DLS) techniques were used to monitor the dynamics of complex formation and particle size. These analysis revealed complexation solution and incubation time of DNA:PEI as relevant factors influencing transient transfection.

DoE-based Response Surface Methodologies were used to find the optimum condition of cell density at the time of transfection ( $1.5 \cdot 10^6$  cells/mL), DNA ( $2.1 \mu\text{g/mL}$ ) and PEI concentration ( $9.3 \mu\text{g/mL}$ ). Of note, this optimum condition was found according to a maximization desirability criteria simultaneously applied to different response variables, namely cell viability, % of transfection and specific production. This methodology implies to give different weights to each of the three response variables regarding their importance. Under these conditions, a ~60% transfection and  $198 \pm 17$  relative fluorescence units (r.f.u) were achieved. In addition, characterization of the optimum DNA:PEI concentrations showed that small complexes ( $1 \mu\text{m}$ ) were more efficient for the transfection of High Five cells.

# Colour and performance tuning for thin film technologies: Photovoltaics à la carte

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Recently, zero-energy buildings are gaining attention due to the reduction of the energy consumption, sustainable management of energy and harnessing of the solar energy, both visible light and thermal parts of the sun spectrum. Silicon photovoltaic (PV) panels are widely installed, but they have certain drawbacks, including the fact that panels are opaque, heavy and with dark colour. On the other hand, organic photovoltaic (OPV) can be an interesting complementary/alternative technology to traditional silicon due to its tempting features. These include low manufacturing cost, very low energy payback times, compatibility with roll-to-roll, semitransparency and ease colour tunability. Furthermore, OPV could potentially be integrated within some untapped architectonic elements such as windows or façades.

Colour and transparency are thus very attractive features for any emerging PV technology, specially targeting building integrated applications. These traits depend on the absorption of the different layers within the device as well as interference effects and thus is often not easy to predict simply analysing the optical parameters of the active layer materials. For this reason, we developed a theoretical tool to predict the colour and performance of a solar cell and apply it to thin film solar cell technologies. This tool relies on transfer matrix method (TMM) approximation to reproduce light-matter interaction. This lead to simulate transmission and reflection spectra of the complete device. Then, CIE coordinates are calculated by combining the calculated transmittance, the model to predict how human eye perceives colours and the spectrum of the light source. Additionally, CIE chromaticity diagram are used to represent colour CIE coordinates of the considered system. Finally, the reverse problem, i.e. finding the appropriate material and device geometry that results in a desired colour, will also be discussed.

## Flexoelectricity in Bones

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Bones have been known to generate electricity under pressure since Fukada and Yasuda's seminal measurement of bone piezoelectricity in 1957. This piezoelectricity is thought to be essential for bone's self-repair and remodelling properties, and its origin is attributed to the piezoelectricity of collagen (the main structural protein of bones). However, since the discovery of flexoelectricity, it is known that strain gradients can also generate voltages in materials of any symmetry. Here we have detected and quantified the flexoelectricity of bone and bone mineral (hydroxyapatite), and determined that flexoelectricity can account for bone's electrical response to inhomogeneous deformations. In addition, we have used the flexoelectric coefficient of hydroxyapatite to calculate the (flexo)electric fields generated by cracks in bone mineral. Crack-generated electricity has been found to be large enough to be able to induce osteocyte apoptosis and thus initiate the crack-healing process, indicating a central role of flexoelectricity in bone damage repair and remodelling.

# Nanomechanical sensing based on 2D colloidal diffraction gratings

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In the last years, nanomechanical sensors have become an emerging and promising technology for sensing and biosensing applications, due to their small size, fast response, high sensitivity and their compatible integration into “lab-on-a-chip” devices. These properties make nanomechanical sensors an especially interesting tool for the diagnosis of diseases where the simultaneous detection of several analytes is mandatory to achieve an appropriate diagnosis and treatment. However the multiplexed capability for monitoring several nanomechanical transducers (each one associated with the detection of a specific compound) still present some limitations related mainly with the integration of the read-out methodology when working with an array of transducers (alignment, power,...).

To solve this limitation, we propose the colorimetric detection of nanomechanical bending. We present the development of polymeric nanomechanical biosensors (membranes or microcantilevers) with integrated diffraction gratings based on 2D colloidal crystals. We explore and exploit the white light diffraction to achieve a power-free array of membranes that change their reflective colour depending on the surface stress change (bending) produced on each sensor. The transducer bending will induce a change on the angle of incident of light and a deformation of the grating (increase or decrease of the pitch for large bending).

We performed a study of the optimum membrane dimensions to maximize both the mechanical response and the colour change associated, when a surface stress-strain change is produced. Polymeric materials, besides being cheap and easily nanostructured, present a much lower Young’s Modulus compare with standard nanomechanical materials such as silicon, which will increase the bending response. Experimentally, the arrays of membranes were fabricated by infiltrating 2D colloidal crystals of polystyrene nanoparticles with Polydimethylsiloxane (PDMS). The membranes were fixed and integrated into a microfluidic system. The colour of each membrane, due to the light scattering, was analysed by UV-visible spectrometry and image analysis looking to develop an integrated multidetection system based on a smartphone reading. We demonstrate the suitability of this approach for the detection of nanomechanical bending induced by the adsorption of elements on the sensor surface.

## High performing OFETs fabricated by BAMS: response under mechanical stress

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Organic Field Effect Transistors (OFETs) can be found in a large number of promising applications such as displays, sensors or small integrated circuits. However, to make organic electronics competitive with their inorganic counterparts, a simple, cheap and scalable solution technique that can give rise to highly crystalline and homogenous semiconducting films is needed. In this work,<sup>1</sup> we report the use of the Bar-Assisted Meniscus Shearing (BAMS) technique for the fabrication of high performance OFETs based on various benchmark p-type organic semiconductors and polystyrene. Furthermore, on the area of flexible electronics, the relationship between morphology and OFET response under mechanical stress (elongation and compression) has been investigated.<sup>2</sup>

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## Charge-density-wave phase interplay in single-layer NbSe<sub>2</sub>

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We present density functional theory (DFT) based studies on the charge-density-wave (CDW) state of single-layers NbSe<sub>2</sub>. We investigate the band structure and Fermi Surface of the single-layer NbSe<sub>2</sub> in order to dismiss the Fermi Surface nesting as possible origin of the CDW phase formation. We calculate the phonon dispersion show the softening of an acoustic mode and reveal a tendency for a reconstruction of a 3x3 supercell in the NbSe<sub>2</sub> single-layers. We follow the evolution of the phononic modes by doping with either electrons or holes. Finally, we present the stability of different CDW phases as a function of the mentioned doping and compare the calculated STM images with the experimental ones.

# Functionalized bacterial nanocellulose for epithelial regeneration

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Nanocellulose (NC) of microbial origin is a biopolymer synthesized and secreted by several bacterial species. NC forms a stable 3D-network comprised solely of pure cellulose nanofibres. NC has unique properties that make it a promising candidate material for tissue regeneration: it has high liquid holding capacity, it is flexible and porous and, importantly, its characteristics can be finely tuned during and after its biosynthesis. Thus, our main goal is to exploit NC as a novel and versatile biomaterial for the regeneration of different kinds of epitheliums.

I will show our first steps towards the development of bacterial nanocellulose patches for epithelial regeneration. Firstly, I will present in vitro biocompatibility studies performed with different bacterial nanocellulose membranes. Then, I will show a specific example of NC functionalization with TiO<sub>2</sub> nanoparticles (NPs). These NPs are commonly incorporated in personal care products as UV filters or whitening agents. When functionalized with TiO<sub>2</sub> NPs, nanocellulose films acquire Ultra Violet (UV)-blocking capacity and could be used to protect sensitive epitheliums from the damaging UV-radiation emitted by the sun. I will describe how the efficacy of this NC-based solar filter was tested using a cellular model and a solar simulator.

## Photothermal activation of MOFs using a UV-Vis light source

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One of the main features of crystalline Metal-Organic Frameworks (MOFs) is their porosity, which allows using them for myriad applications such as gas storage, catalysis, sensing, biomedical fields, among others.<sup>1,2</sup> However, using these materials for all these applications requires their previous activation, which consists on removing the solvent molecules located inside their pores or coordinated to the metal centres. To date, the most common activation methodology entails first a solvent exchange step, where the solvents are replaced for more volatile ones, followed by a thermal evacuation of the solvent molecules applying heat and vacuum. Although other activation methods have been developed<sup>3</sup> (e.g. supercritical CO<sub>2</sub>, freeze-drying), most of them are still solvent-, time- and energy-demanding processes.

In this communication, we present a novel activation technique based on the localized light-to-heat conversion induced by directly irradiating MOF powders using a UV-Vis lamp. This photothermal process is based on the light absorption of the organic ligands and the ligand to metal charge transfer bands (LMCT) in the irradiation range (300-650 nm), after which the excess of vibrational energy due to electron relaxation is released as heat. By following this method, we demonstrate the activation of a series of well-known MOFs, including HKUST-1, ZIF-8 and -67, UiO-66 and -66-NH<sub>2</sub>, CPO-27-M (M=Zn, Ni, Mg), IRMOF-3 and Fe-MIL-101-NH<sub>2</sub> in only 30 min and suppressing the need for long solvent exchange procedures. This short activation times are achieved thanks to the homogeneous photothermal effect acting locally in the framework, allowing an improvement of the heat diffusion.

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# Physical properties of nanostructured, liquid assisted grown, epitaxial $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ superconducting films

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Being one of the most profoundly studied fields in modern physics, superconductivity yet remains a topic of global interest. At present, Low Temperature Superconductors (LTS) govern the major part of market applications (e.g. Nuclear Magnetic Resonance Spectroscopy (NMR) and High Magnetic Fields) although High Temperature Superconductors (HTS) exhibit highly increased performances in their superconducting state. What is still limiting HTS to enter a broad market to the point of commercialization of superconducting tapes is its high cost/performance ratio.

To address this issue, we are developing a novel growth technique to fabricate low-cost, high throughput Coated Conductors (CCs)<sup>1</sup> incorporating  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  (YBCO) as superconducting layer. Growth rates up to 50 nm/s, surpassing any conventional method by one order of magnitude, are confirmed and higher values foreseen. The technique is based on Chemical Solution Deposition (CSD) which is known for its technological simplicity and upgradability to integrate smart solution deposition (such as inkjet printing and additive manufacturing).

First low-temperature measurements reveal high critical temperatures and current densities proving the relevance of the developed approach.

Besides introducing principal ideas of the novel growth route, the talk aims to give an overview over the main measurement techniques used to optimize growth parameters and value the state and quality of our films: We perform in-situ growth analysis by means of synchrotron X-ray diffraction to follow the evolution of all involved phases during growth; Oxygenation kinetics are studied by relating charge carrier densities (via Hall effect measurements) with X-ray diffraction results; A deep study of how microstructure affects the superconducting properties is carried out through the interplay of electron transmission microscopy and low temperature critical current measurements.

## *Acknowledgements*

The research leading to these results has received funding from ERC (EU ERC-AdG- 2014-669504ULTRASUPERTAPE project) and Programa excelencia Severo Ochoa SEV2015-0496.

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# Carbon/sulfur nanotubes composites as cathode materials for high performance Li-S batteries

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Today, the modern world cannot be described without considering lithium-ion batteries. Current concern about limited energy resources, coupled to the need to decrease greenhouse gas emissions, has brought the need to consider renewable energies at a large scale together with the use of hybrid and electric vehicles. Among the various energy conversion/storage systems proposed over the two last centuries, electrochemical storage and more specifically batteries seem to be very well positioned to satisfy these needs, but research to meet the application requirements is still an imperious need.<sup>1</sup>

Lithium-sulphur (Li-S) batteries are regarded as one of the next-generation energy storage systems due to the extremely low-cost sulfur and their high energy density.<sup>2-4</sup> The price of sulphur per metric ton was as low as \$160 USD in 2012.<sup>5</sup> The theoretical capacity of sulphur is 1672 mAh/g (calculated based on  $S^0 \leftrightarrow S^{2-}$ ). Coupled with the average operating voltage of a Li-S cell (2.15 V vs  $Li^+/Li^0$ ) and the theoretical capacity of a pure lithium anode (3862 mAh/g, calculated based on  $Li^+ \leftrightarrow Li^0$ ), the energy density can be estimated as high as ~2500 Wh/kg, which is an order of magnitude higher than that of traditional Li-ion batteries. Although Li-S batteries possess many advantages, low active material utilization, capacity degradation, self-discharge, poor Coulombic efficiency, poor cycle life, and electrode volume expansion are still the challenges remaining with the Li-S cells.<sup>2, 6, 7</sup>

The objective of this work is to investigate the fundamental chemistry of sulphur composites and develop new functional electrode materials and architectures for high energy, low cost Li-S batteries.

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# **Electron beam lithography patterning for a cell traction force microscope**

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Mechanical characterization of living cell plays an important role in the study of many different processes which take place in this kind of biological systems. The determination of the force that a cell can apply is important as it may affect its migration or its differentiation, among others.

Here, we developed a Traction Force Microscope (TFM) which allows the quantification of the cell migration forces. Previous works from other authors have presented a TFM consisting of a substrate with a random distribution of embedded beads, which makes measurement more difficult and increases errors. This TFM is based on an array of periodically-spaced dots printed with a polydimethylsiloxane (PDMS) stamp. The PDMS stamp consisted in vertical nanopillars of 200 nm of height and 160 nm of diameter. The top surface of the nanopillars was initially inked with a quantum dot solution and then was stamped on a substrate in which living cells will grow. The PDMS stamp was replicated from a silicon mold, which was previously fabricated with the Electron Beam Lithography (EBL) technique.

When a cell exerts a force on the substrate, the position of the printed spots in this part of the substrate will be laterally displaced. The deformation of the substrate can be correlated to the exerted forces. Due to it is a periodical spot pattern, it is easy to notice this change, and from this shift, we are able to calculate the applied force by the cell.

## Optomagnonical cavities

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The ability to control magnetism has played a major role in the development of communication technologies. Today's research focuses on the manipulation of individual or collective spins. In particular, the use of collective excitations in magnetically ordered materials, magnons, which are considered very useful by their high tunability, whose range covers from the MHz to the THz.

We demonstrate the detection of magnon modes through optical transduction using a non-magnetic whispering gallery mode resonator. The strategy explored in this experiment is about trying to detect magnons on planar YIG samples that do not form a cavity. We use glass microspheres that do not show a magnetic behaviour. The spheres have high quality factor  $Q=10^5$  which allow to use them as a sensor for coupling and collecting the evanescent light interacting with the magnetic material. This method offers a new range of possibilities to detect magnon resonances in ferromagnetic materials. The fact that a spherical magnonic cavity is not required also allows for the possibility of developing on-chip magnon technology.

## **Dependence of the accumulation function on the regularization parameter in the MFP reconstruction technique**

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In the study of thermal transport phenomena at the nanoscale, it is usual to introduce a spectrum-averaged phonon mean free path (the gray-MFP approximation). However, recent reports have shown that the use of a single-averaged MFP may be inadequate. The analysis of the contribution of heat carriers with different MFP to the total thermal conductivity is key to understand the role that different physical phenomena play in the reduction of thermal conductivity in nanostructured materials.

In the MFP reconstruction process, the election of the regularization parameter is of great importance to obtain an adequate suppression function that relates the bulk thermal conductivity and that of the nanostructure. In this work, we study the criteria for choosing a value for the regularization parameter and the influence of this election in the final result of the MFP reconstruction. This process is then applied to calculate the thickness-dependant suppression function for thermal conductivity in Silicon membranes.

## Structure of C<sub>60</sub>/ClAlPc systems on Au(111) at submolecular scale

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The study of organic-organic interfaces, in particular donor-acceptor heterojunctions, has gained a lot of interest in the last years due to their important role in organic electronic devices as organic solar cells.<sup>1</sup> Thus, the fundamental study of these structures at the nanoscale is of great importance. By means of self-assembly and self-organized growth paths in Ultra High Vacuum (UHV) conditions, two dimensional organic layers can be constructed and examined by Scanning Probe Microscopy techniques. In our work, the system under study is the phthalocyanine chloroaluminium (ClAlPc) donor and the fullerene (C<sub>60</sub>) acceptor molecules. ClAlPc presents an interesting case of study as, when sublimated on Au (111), self assembles in organized layers with two clear configurations: Cl-Up and Cl-Down.<sup>2</sup> Thus, this two molecule system provides us with insight on how the structural properties as order and molecular orientation can influence and affect the adsorption and self-organization of the C<sub>60</sub> molecule on the ClAlPc/Au(111) system. The structure at the molecular and sub-molecular level has been investigated for different surface coverages by UHV STM/nc-AFM. These measurements reveal that when the C<sub>60</sub> is sublimated onto the first ClAlPc monolayer, it assembles in a structure that replicates one of the main orientations of the ClAlPc/ monolayer. Remarkably, C<sub>60</sub> does not adsorb onto two layers ClAlPc films. This has been further proved by obtaining ClAlPc films consisting of a complete first layer and an incomplete second layer. In such a system, for a low C<sub>60</sub> coverage, the C<sub>60</sub> is only found to adsorb on the first layer. When the C<sub>60</sub> coverage is increased, non-crystalline clusters of the molecule are formed. Finally, in order to explore the changes in the local work function, comparative measures of local contact potential difference (CPD) have been made.

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## **Electrical characterization of TiN/Ti/HfO<sub>2</sub>/W resistive switching devices**

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TiN/Ti/HfO<sub>2</sub>/W devices have been fabricated and their resistive switching (RS) characteristics have been assessed by sequential voltage ramps and trains of pulses. The analysis of the obtained results indicates an asymmetric bipolar RS behaviour with two very well-defined resistance states, High Resistance State (HRS) and Low Resistance State (LRS), and good reliability in large sequences of voltage sweeps and pulse-train cycles. In addition, by varying the electrical parameters of the experimental measurements, the multilevel capability of the devices has been analysed, and the obtained results suggest that the studied devices can be employed as multibit memories or electronic synaptic devices in neuromorphic circuits.

# Molecular dynamics simulations of a novel vesicular system for nanomedicine applications

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In the last years, we have been developing novel mixed surfactant-sterol vesicular systems (called Quatsomes) for nanomedicine applications.<sup>1</sup> These Quatsomes are stable and homogeneous vesicles with a particle size of 70-100nm. A prototypical example of Quatsome are vesicles formed by a 1:1 mixture of CTAB surfactant and cholesterol in water, which are useful for the topical delivery of pharmaceutical active ingredients.<sup>2</sup> Nevertheless, for other applications involving intravenous administration CTAB is not a suitable surfactant due to its toxicity.<sup>3</sup> In order to be able to use Quatsomes for these applications, we are developing combined theoretical and experimental studies to identify suitable alternative surfactants. These studies will also show how the properties of the supramolecular vesicle (which contains both the surfactant and cholesterol) depend on the molecular details of the selected surfactant.

In this contribution, we discuss in detail the particular case of vesicles made of myristalkonium chloride (MKC) surfactant and cholesterol. It was found experimentally that the presence of salt in solution (NaCl) is essential to achieve stable vesicles made of MKC/Cholesterol but also an excess of salt makes the vesicles unstable. Hence, these cationic vesicles can exist only in a certain, appropriate range of salt concentration. On the contrary, in the case of CTAB/Cholesterol system, Quatsome vesicles were already formed in pure water and are stable in a wide range of salt concentration. In order to understand this puzzling effect, we performed extensive atomistic Molecular Dynamic simulations with the MKC/Cholesterol system in water and in presence of NaCl salt at different concentrations. High-level DFT Quantum Mechanics calculations were used for the parameterization of the Force Fields employed in our Molecular Dynamics simulations.

Our simulations predicted that anions not only adsorb onto the membrane surface but also some of them penetrate in the membrane structure, being an integral part of this cationic vesicle. At concentrations of 100 mM of NaCl our simulations correctly predict the formation of stable bilayers, whereas at concentrations of 500 mM of NaCl the bilayer structure is no longer stable and vesicle formation is not possible.

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## **Guiding pattern options to direct the self-assembly of block copolymers**

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The use of block copolymers for lithography applications has attracted significant attention in the last years because it is an interesting bottom-up technique for patterning with critical dimensions in the range from 5 to 25 nm.

Block copolymer thin film spin coating and annealing leads to a microphase separation process which, however, lacks the capability of inducing long-range order in the system. Different strategies can be pursued to order the block copolymer domains on a large length scale and to assemble the material in lithographically relevant structures. Features capable of inducing long range order in block copolymer films are called guiding patterns.

We give an overview over a variety of the most widely used guiding pattern fabrication techniques and explain the ordering mechanisms of each one of them based on examples from our lab.

## Understanding ferroelectricity in epsilon-Fe<sub>2</sub>O<sub>3</sub> films

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Over the last decade, unprecedented efforts have been devoted to searching for suitable multiferroic materials with notably cross-coupled ferromagnetic and ferroelectric orderings, which are highly attractive from both the fundamental and the technological point of views. Thin epitaxial films of the polar ferrimagnet  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub>, recently reported to be ferroelectric, enlarge the selective group of very few single-phase magnetoelectric multiferroics at room temperature.<sup>1</sup> However,  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub> films present a small magnetoelectric coupling and the mechanism of ferroelectric switching is still not understood.

To further investigate the origin of ferroelectricity in  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub> we stabilized this phase on different surfaces by pulsed laser deposition. In particular  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub> (001) films were prepared on AlFeO<sub>3</sub> (001)/LaNiO<sub>3</sub> (111)/Nb:STO (111) and on Fe<sub>3</sub>O<sub>4</sub> (111)/MgAl<sub>2</sub>O<sub>4</sub> (111) to be compared to previously studied ferroelectric  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub> (001) films on AlFeO<sub>3</sub> (001)/Nb:STO (111).<sup>1</sup> The films were characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM) and atomic force microscopy (AFM) and piezoresponse force microscopy (PFM). XRD shows an enhanced crystallinity of the films with LaNiO<sub>3</sub> (111) layer. But surprisingly, PFM measurements and TEM analysis with an in-situ application of switching voltages did not reveal any sign of ferroelectricity. This points to a non-conventional origin of ferroelectric switching in  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub>, which might be related to twin boundaries or domain structures.

### *Acknowledgements*

We acknowledge the support by the “Severo Ochoa” Programme for Centres of Excellence in R&D (SEV- 2015-0496), the Generalitat de Catalunya (2014SGR213) and the Chinese Scholarship Council (fellowship 201606070094 to Z.M.).

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# Evaluation of the nano-bio interactions between Au-NPs and *Caenorhabditis elegans*

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*Caenorhabditis elegans* (*C. elegans*) is a relevant animal model in different subjects from genetics to toxicology. Their experimental features, including easy and inexpensive maintenance in the laboratory, short lifespan, large number of offspring, transparency and small body size, offer significant advantages over more complex model organisms to perform a preliminary screening of nanoparticles for biomedical applications in the chemical laboratory.<sup>1</sup>

Gold nanoparticles (Au-NPs) are promising inorganic nanoparticles for nanomedicine due to their interesting properties including their chemical inertness, intense surface plasmon resonance (SPR), easy surface functionalization and easy tuning of size and shape. Many applications as theranostic, diagnostics and targeting agents are currently under investigation.<sup>2</sup>

Here we made a series of studies in *C. elegans* including the analysis of toxicity endpoints, the investigation of nano-bio interactions by means of imaging and chemical techniques, and molecular analysis of NP-responsive biological responses. To this aim, we evaluated two different sizes of citrate-coated Au-NPs, 11 and 150 nm. We report that 11-nm Au-NPs are more toxic than 150-nm Au-NPs, however acute exposure up to 100 µg/ml is still safe. We investigated the biodistribution of both types of Au-NPs, and found they were contained in the intestinal lumen of *C. elegans* with no apparent endocytosis, in contrast to previous work.

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**Poster Presentations**

## **Ab initio study of oxygen vacancies in YSZ for gas sensor**

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The monitoring of gases with solid state sensors has become a well-established practice in industry. There are many categories of gas sensors, among them oxygen gas sensors are one of the basic gas sensors with purpose of measuring oxygen concentration in auto mobile exhaust to control the pollution. In this project, the main goal is to develop atomistic models of yttria stabilized zirconia (YSZ) which is promising material for electrolyte in gas sensors owing to its high ionic conductivity.

Due to huge configuration of structure with different vacancy defects, we deduce these structures using symmetry. At first step, we are going to relax all the structures to find out each defects formation energy using SIESTA package within framework of density functional theory (DFT) afterward we try to find out migration energies of vacancies in different configurations. This step will be done by nudge elastic band (NEB) method in SIESTA. After bulk calculations, we build the slab and investigate the different configurations with appropriate surfaces. Next, we introduce the electrodes to capture more realistic picture for evaluating the migration energies.

## Activation of microporous Co-CB MOF by supercritical CO<sub>2</sub>

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Metal organic frameworks (MOFs) emerged as a class of solid-state hybrid materials with applications in adsorption, due to their high porosity as well as surface area. Nevertheless, the handling and activation of MOFs are crucial factors affecting the surface area and pore volume. This is particularly important for MOFs that are susceptible of collapse after solvent elimination. It has been demonstrated that scCO<sub>2</sub> activation can sometimes preserve the integrity of MOFs to a larger extent than vacuum evacuation. In this work, a microporous MOF of Co is activated following two different approaches.

## Stable perovskite solar cells employing oxide interlayers

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An ideal interlayer for high efficient Organic (OPVs) and Perovskite Solar Cells (PSCs) should meet the following requirements: a) good compatibility with the active layer, b) optical transparency, c) good conductivity, d) good charge transport properties and e) processability. Transition Metal Oxides (TMOs) have emerged as promising interlayers for OPVs and PSCs. They confer high stability and moisture resistant properties, the appropriate work function, high transparency and are compatible with solution-processable techniques required for the fabrication of OPV and PSCs. Comparison between interlayers made of TMOs and organic semiconductors (i.e. poly(3,4-ethylenedioxythiophene):poly(4-styrenesulfonate), PEDOTSS) have resulted in devices with similar or enhanced efficiency and superior lifetimes. TMOs have been applied as electron (ETM) and hole transport materials (HTM), mostly as simple binary oxides (i.e. TiO<sub>2</sub>, ZnO, NiO, CuO<sub>x</sub>), but complex (i.e. ZnSnO<sub>4</sub>, SrTiO<sub>3</sub>) and doped oxides (i.e. Cu-NiO or Cu-CrO<sub>x</sub>) are currently breaking ground demonstrating device stabilities of thousands of hours. In this work, we present our most recent results on the application of semiconductor oxides in Perovskite solar cells and the effect of device stability.

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# Developing of 3D printing of complex ceramic devices for energy application

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Manufacturing of functional ceramic materials is limited, in general, by the production of sheets by tape casting or screen printing and tubes by extrusion. On the devices based on functional ceramics which suffer from these limited shapes, there are the solid oxide cells (SOFCs: Solid Oxide Fuel Cells whose aim is to convert the chemical energy stored into the hydrogen bond and SOECs: Solid Oxide Electrolyser Cells, which produce oxygen and hydrogen starting from water). Moreover, the SOFCs are stacked to obtain higher output current; this is done using metallic bipolar plates as interconnectors that are sealed to the ceramic cells. The presence of these joints promotes weak points on the final system, whose manufacturing requires more than a hundred productive steps, many of them involving manual processes. On the other hand, the performance of these devices is strictly related with their active area, which is also limited by the tubular or flat shapes. All these limitations result in a difficult entry into the market which demands to achieve low production costs and high performance and durability.

The stereolithographic 3D printing allows producing ceramic pieces with complex desired shape and opens new frontiers to the high active area designs for the fuel cell. At the same time, the realization of a multi-material system in few steps will decrease the manufacturing costs and it will produce monolithic devices with more robustness and durability.

The present work presents a preliminary study of 3D-SLA printing to achieve new geometries and multi-material printing of SOFC/SOEC devices using YSZ as printed SOC electrolyte material.

## *Acknowledgments*

The authors want to acknowledge the 3D-MADE project (ENE2016-74889-C4-1-R), the CELL3DITOR project (FCH-02.6-2015) and the collaboration of 3DCeram in the printing process.

# Role of oxygen exchange kinetics in the engineering of carrier concentration of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ films

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The superconducting properties of cuprates are crucially influenced by its oxygen content. Achieving optimal oxygen doping in YBCO films is still an open issue and its optimization a main goal of this work. The oxygenation kinetics is strongly influenced by microstructural and morphological features of the films, which strongly defer depending of the growth technique. These kinetic effects, as molecular oxygen absorption, dissociation and atomic diffusion within the bulk, can be addressed by in-situ electrical conductivity relaxation measurements, to achieve a full control of the final carrier concentration of YBCO films and coated conductors.

We show that in-situ electrical conductivity measurements are a very useful tool to analyse the oxygenation process of YBCO films. We monitor the mechanisms of oxygen incorporation and exit in standard and nanocomposite CSD and PLD YBCO thin films during post annealing of grown films. This analysis allowed us to determine the dependence of the oxygenation rate of in- and out-diffusion (bulk and surface) on several processing parameters, as the  $\text{O}_2$  partial pressure, temperature and gas flow and obtain time constants and activation energies for each case. Our results demonstrate that the oxygenation of the thin films studied, is limited by the involved surface reactions. We show that catalytic agents deposited on the surface, strongly accelerate the oxygen exchange and allow us to work at lower oxygenation temperatures, leading to higher oxygen contents. With a deep understanding of the oxygenation process we can properly engineer the carrier concentration and change the oxygen content in our films from the underdoped to the optimal doped and even the overdoped regime, as monitored by Hall effect and c-axis lattice parameter measurements.

Therefore, we can properly study and analyse the correlation of the doping level of YBCO thin films and the superconducting properties as the critical temperature and especially the critical currents, with the aim to maximize the latter.

## Heavy metals detection using screen printed carbon electrodes

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Heavy metals are chemical compounds that are non-biodegradable and pose a severe threat to human health and environment. These compounds are spread in the environment at higher concentrations due to human activities like mining, smelting etc. These low density toxic compounds can alter the functioning of cellular components in the living organisms by binding to specific sites and interfering with the natural biochemical processes. Considering the severity of their effects on humans and other living organisms, INCATCH H2020, a European project aims at finding easy, compatible and cost-effective methods to detect these metals from river waters. In this work, we report an easy to use electrochemical sensor for detection of Copper, Cadmium and Lead in a flow-based system using home-made screen-printed Carbon electrodes. The system performance and detection limits for such metals in the absence and presence of interference are presented. Low LODs obtained for Cd, Cu and Pd was 3.72, 0.38 and 0.006ppb respectively.

# **Fabrication of FinFETs by directed self-assembly of block copolymers and electron beam lithography**

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The continuous demands from industry for more powerful electronics have pushed nanofabrication methods to the limit. With the upcoming rise of the Internet of things (IOT), billions of nanoelectronic devices will need to efficiently exchange data, leaving no room for performance saturation due to miniaturization limitations.

Novel lithography techniques are being developed to fabricate the most advanced transistors in sub10 nanometer nodes, but while some methods lack throughput, others bring highly increased costs due to complex manufacturing. Directed self-assembly (DSA) of block copolymers (BCPs) is presented as a complement to traditional lithography processing techniques, offering high resolution and throughput at an affordable price.<sup>1</sup>

BCPs are macromolecules that consist of two or more polymer chains covalently linked to each other. Due to force interactions between these different chains, and depending on the molecular weight of each segment, BCPs can form different nanometer-scale periodic structures<sup>2,3</sup> that can be then transferred to substrates.

In this work we present a process, based on DSA of BCPs, that enables the creation of nanometerscale single-crystal silicon wires which, after gate structuring, can serve as the base blocks for multigate FinFET arrays. First, poly(styrene-*b*-methyl methacrylate) (PS-*b*-PMMA) is direct self-assembled into vertical lamellae on a prestructured guiding pattern. Second, the DSA pattern is transferred into the silicon substrate by reactive ion etching. Once the fins are formed, conventional CMOS fabrication methods can be used for the definition of the transistor gate stack, terminals and contacts.

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# Electrodes based on biochar – application in the determination of phenolic compounds

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Biochar is a carbonaceous material obtained by biomass pyrolysis in a low amount of oxygen. This highly porous material presents surface functional groups, which is very interesting from the analytical point of view, due to the high adsorption capacity of organic and inorganic compounds.<sup>1</sup> By the chemical activation process of the carbonaceous surface it is possible to increase the amount of oxygenated and nitrogenous biochar functional groups. This can be accomplished by exposing the material to oxidizing or reducing agents under refluxing reaction.<sup>2</sup>

In this work, castor bean biochar was submitted to chemical treatment with HNO<sub>3</sub> under optimized conditions of refluxing: temperature of 60 °C and reaction time of 3 h. The material obtained was additionally “decorated” with metallic nanoparticles for the development of electrochemical sensors. Thus, palladium (PdNP) and gold nanoparticles (AuNP) were synthesized and incorporated into the activated biochar. Therefore, the materials were characterized morphologically and applied in the modification of different carbon-based electrodes: Carbon paste electrode modified with biochar, biochar-PdNP, and biochar-AuNP. Comparatively, electrodes based on mesoporous carbon and graphite (without modification) were made. The electrodes were electrochemically evaluated after the spontaneous preconcentration (open circuit) of the following phenolic compounds: catechol, 4-ethylcatechol, 4-ethylphenol and 4-ethylguaiacol. Analytical calibration curves were obtained for each analyte with the electrodes evaluated. It was possible to observe that the electrodes modified with biochar had a better adsorption capacity of the evaluated compounds, which reflected in a better detectability and sensitivity, with limits of detection in the concentration range of nanomolar. This allows the electrodes to be applied in the determination of phenolic compounds with high detectability in real samples.

The next step of this work concerns the development of a voltammetric electronic tongue for the determination of such phenolic compounds in wine samples. This determination is of great interest in the wine field, as it permits the detection of an important defect during vinification, the Brett character.

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## Characterization and added value to bio-oil derived from Sansa

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The aim of this project is to explore the potential of bio-refinery as an alternative way of obtaining energy and chemicals from residues. Sansa, also known as two-phase olive mill wastewater (TPOMW) is a residue obtained from olive oil production. TPOMW contains different high value compounds like antioxidants (present in olives). Studies of the residues treatment have been done both, for environmental issues and economic benefits, which allowed companies to take profit of the composition of TPOMW by the use of bio refinery processes. This procedure is based on breaking macromolecules into small ones. Moreover, the thermochemical treatment allows a previous separation, obtaining a clean liquid phase of minerals and salts, which remain in the solid phase. The bio-oil is composed of two phases, a viscous one and a fluid one. Viscous and liquid phase are composed of fatty acid, methyl esters of fatty acids and poly-methoxyphenols, and acetic acid, sugars and poly-methoxyphenols, respectively. Both phases have been characterized by measuring pH, water content (Karl-Fischer method), composition (Gas Chromatography – Mass Spectroscopy) as well as their solubility in different solvents. Besides, a method to separate the high value compounds present in the bio-oil phases is studied. The method is based on extractions at different pH using different solvents. Overall, the results showed that families of compounds can be separated using this methodology. The separation of these compounds could constitute a game changer in the economy of a wide variety of industrial companies.

## **Magnetic properties of nanoporous Co-Pt micropatterns synthesized by micelle-assisted electrodeposition on photolithographed substrates**

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Miniaturization of magnetic materials has been extensively investigated due to the significant size effects observed on their magnetic properties and the resulting technologically relevant applications. Herein, electrodeposition combined with optical photolithography has been utilized to fabricate magnetic microstructures for applications in spintronics, recording media and other eventual magnetically-actuated devices.

Focused on this challenge, nanoporous Co-Pt microstructures have been successfully synthesized onto pre-lithographed Cu(70 nm)/Ti(10 nm)/Si substrates. Co-Pt actually constitutes one of the most currently used material in magnetic storage systems. Arrays of cylindrical holes, triangles, squares and donuts from 50 to 5  $\mu\text{m}$  in diameter and 5  $\mu\text{m}$  in height were first patterned by Optical Lithography (OL). Subsequently, the patterned area was used as template for the potentiostatic electrodeposition of the Co-Pt microstructures from a plating bath containing metal chloride salts and Pluronic P123 tri-block copolymer. Scanning electron microscopy and Energy-dispersive X-ray spectroscopy (EDX) analysis showed well-formed Co-Pt 3D nanoporous microstructures with a Co-rich composition. The nanoporosity was induced due to the presence of P123 in the bath which tends to form nanoscale micelles that act as a structure directing agent during electrodeposition. Interestingly, magnetic measurements reveal variations in the the coercivity ( $H_c$ ) depending on the micro-structure's size, observing an increase on the coercivity as the structure size decreases. Furthermore, a drastic reduction of the coercivity ( $H_c$ ) was observed at room temperature by subjecting the microstructures to an electric field (i.e., magneto-electric effect) using an anhydrous electrolyte. This change in  $H_c$  could, in principle, be attributed to a purely magneto-electric effect (accumulation of electrostatic charges at the surface of the pore walls) or to a redox reaction, although the latter would not be favoured due to the lack of water in the electrolyte. This behaviour could be exploited in a wide range of fields such as spintronics and energy-efficient memory operations. Our study constitutes one of the first works in which micelle assisted electrodeposition and optical lithography are combined to prepare micrometer size nanoporous magnetic materials, with adjustable magnetic properties, that could boost a wide range of technological applications.

## Label-free impedimetric aptasensor for Codeine detection

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This research develops label-free aptasensors for Codeine (Cod) detection using electrochemical impedance Spectroscopy (EIS) technique. EIS is a simple, high-sensitivity, low-cost and rapid transduction principle to follow biosensing events that take place at the surface of an electrode. Besides, the EIS technique is also capable of showing response at very low concentration levels.

Codeine (3-methylmorphine) is an alkaloid separated from opium. This small molecule is extensively used to treat mild to moderate pain and cough suppression in clinics. Despite its medical applications, the abuse of codeine can also create health risks. For this reason, it is very important to find a high sensitive, cheap and rapid method for its detection.

In recent years, a widely variety of conventional methods for the detection of codeine have been developed such as high-performance liquid chromatography, capillary electrophoresis, gas chromatography-mass spectrometry, UV spectrophotometric techniques among others. These methods are expensive and need complex procedures. For this reason, there is a need to develop rapid, cheap and effective devices for detection. To overcome this problem aptasensors is a good alternative.

To achieve the main feature of this work, screen-printed electrodes modified with carboxyl functionalized multi-walled carbon nanotubes (MWCNT-COOH) obtained from Drop Sens (Oviedo, Spain) were used as platforms for impedimetric aptasensing. A covalent immobilization of aminated DNA target using carbodiimide chemistry was performed. In this case, the covalent binding is produced by first electrochemical grafting. Electrochemical grafting consists of anchoring 4-aminobenzoic acid molecules to the electrode surface through diazonium salt reaction and C-C bond formation. This step leaves benzoic acid moieties exposed to the solution and can be used to immobilize biomolecules that are amino terminated. After that, a blocking step is performed using polyethylene glycol as blocking agent; the label-free assay to detect Cod consists on a simple incubation step with the sample.

To conclude, the developed method could be a useful and promising platform for codeine detection in many applications. In addition, the use of EIS technique does not require any additional and/or labelled species for the transduction. Thus, this detection technique can be used for designing label-free protocols avoiding more expensive and time-consuming assays.

# Effects of post- and in-situ heat treatments on sputtered copper-aluminium-nickel shape memory alloys

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Thin film sputtering is an appropriate method that allows the manipulation of structure of materials that are to be used in MEMS/NEMS applications. It is a known fact that materials with highly preferentially oriented structures exhibit improved properties compared to polycrystalline materials. Therefore, it is significant to discuss the synthesis approaches in sputtering that result in different crystallographic structures. In order to point out this aspect, two types of sample preparation methods to obtain shape memory properties in Cu-Al-Ni system were implemented: One is the preparation of 1.25 micrometer thick multilayers of Cu-Ni and Al at room temperature consisting of three 70 nm thick Al layers between four Cu-Ni layers two of which at the bottom and on top are 173.5 nm thick while the others are 347 nm thick. These multilayers were subjected to subsequent heat treatment at 800 °C for 1 hour and quenching in iced-water. In the other method executed, co-sputtering from Cu, Al and Ni targets onto MgO(001) substrates with in-situ heat treatment at 650 and 700 °C was carried out. Energy-Dispersive X-ray Spectroscopy (EDX), X-ray Diffraction (XRD) and Transmission Electron Microscopy (TEM) analysis revealed that a slight shift in the composition, from CuAl<sub>14</sub>Ni<sub>4</sub> to CuAl<sub>12</sub>Ni<sub>7</sub> (wt %), results in a phase change, at room temperature, from martensite to polycrystalline austenite in the conventionally quenched multilayers. In turn, the epitaxial relationship MgO(001)[100]/CuAlNi(001)[110] was induced in the CuAl<sub>12</sub>Ni<sub>7</sub> (wt %) films sputtered onto MgO. Growth of (200) textured austenite was attained during in-situ heat treatment at 700 °C while no significant austenite growth was seen in the films grown at 650 °C. In resistance vs. temperature measurements carried out to investigate the shape memory properties in the samples sputtered onto MgO, a slope change between the heating and cooling curves took place for the sample preferentially oriented along the (100) direction which might be indicative of martensitic phase transformation. On the other hand, no change was observed for the sample prepared at 650 °C. Even though it was seen that CuAl<sub>12</sub>Ni<sub>7</sub> (wt %) austenite phase can be obtained by both synthesis methods, preferential orientation was not favored in case conventional post-treatment is applied. Due to the fact that in-situ heat treatment during film synthesis promotes epitaxial growth, it is more suitable to utilize in order to acquire superior shape memory properties in CuAlNi thin films.

# New carborane based dipyridyl linkers for coordination polymers/metal organic frameworks

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*Closo*-carboranes (dicarba-*closo*-dodecaboranes;  $C_2B_{10}H_{12}$ ) are a unique class of boron-rich cluster compounds with desirable properties that could not be explored from carbon-based systems. The incorporation of carborane derivatives into MOFs produces favourable properties such as thermal robustness, varied chemistry and high hydrophobicity.<sup>1,2</sup>

Herein, we have designed and synthesized new disubstituted *m*-carboranylpyridylalcohols (L). Thus, a novel family of coordination polymers (**Figure 1**) was obtained via solvothermal reaction with metal salt, carborane derived ligands and different carboxylic acids. In addition to that, MOF 3 shows potentially high hydrophobicity, thermal stability and controllable chemical properties.

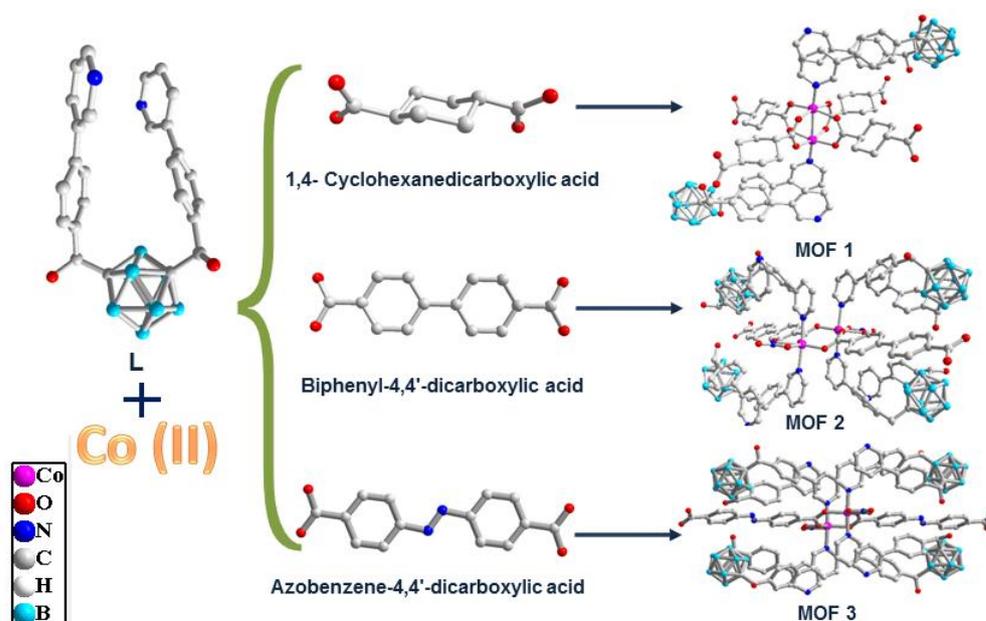


Figure 1. Representation of the new ligand and of the synthesis of MOFs employed in this work

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# Effect of the intercalation of graphite in a metal/graphene contact

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In order for graphene and other two-dimensional materials to become competitive, one of the main technological hurdles that must be overcome is achieving a low contact resistance ( $R_c$ ). For graphene, it is often quoted that an  $R_c$  value lower than  $100 \Omega \cdot \mu\text{m}$  is desirable, while larger values are thought to be a limiting factor on the graphene field effect transistor performance. On the other hand, electron passage from graphite into graphene will suffer the minimum amount of disturbance. Thus, it is conceivable that a graphite/graphene junction would present a significantly low contact resistance. Some experimental observations point along that direction, while in another occasion a graphite/graphene contact has proven superior to using Cr/Au as the electrode. We present results computing, from first principles, the ballistic conductance of a graphene on graphite contact where (a) graphene infinitely extends over the graphite substrate, and (b) graphene has a finite overlap with the graphite substrate. Of course, in real devices graphite would eventually contact some metal in order to decrease electrode resistance. We will also address this, computing the conductance and contact resistance of a metal/graphite/graphene structure, and comparing them to the values obtained for the corresponding structures without graphite.

## *Acknowledgements*

We acknowledge financial support by the Spanish MINECO under Project No. TEC2015 - 67462-C2-1-R (MINECO/FEDER). Also, this project has received funding from the EU Horizon 2020 research and innovation program under grant No 696656, and the DURSI of the Generalitat de Catalunya under contract 2014 SGR 384.

## Trends in sulfur containing species monitoring

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The over exposure of workers involved in decontamination processes in sewage treatment plants and the direct impact in rivers and streams has triggered the alarms. Among others, the wrong treatment of sulphur containing species such as sulphide, sulphate, sulphite and thiosulfate has constituted a global concern. Their presence in the environment above the maximum allowed by the legislation is suspected of causing serious health-risk issues. Thus, it is also interesting to monitor these sulphur species in processes of biological treatment of contaminated water or gases. In this scenario, researchers are developing new methods for their quantification that excel for their selectivity and sensitivity as well as provide fast response in a cheaper manner. Here, the state-of-the-art in the quantification of sulphur containing species is discussed.

# Electrochemical lateral flow devices for the simplification of rapid immunomagnetic-assays

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**Introduction:** Using magnetic beads (MB) allows production of electrochemical immunomagnetic sensors of superior performance than classical immunosensors.<sup>1,2</sup> However, immunomagnetic sensors involve numerous steps and tedious handling. We show that electrochemical lateral flow strips (ELFS) produced by a simple and low-cost screen printing procedure can be used to integrate the washing and detection steps of immunomagnetic assays, contributing to simplify manipulation greatly.

**Methods:** Three-electrode systems were screen-printed on Fusion 5 strips (GE Healthcare). Streptavidin-coated MB (1  $\mu\text{m}$ , Invitrogen) modified with anti-myeloperoxidase (MPO) biotinylated antibodies (Ab, Hytest) were simultaneously incubated with MPO and HRP-labelled Ab (Ab-HRP) for 5 min. MB were confined on the strip using a magnet, flow-washed and detected chronoamperometrically using a commercial TMB substrate solution (Sigma).

**Results:** While screen mesh and ink composition were crucial for subsequent ELFS flow and detection performance, immunoassay electrochemical detection was strongly affected by MB/sample volume and washing solution. Upon optimization, the assay consisted on a single 5-min incubation of sample, MB and Ab-HRP, the reaction mixture was directly pipetted on the ELFS, and washing and detection were performed while MB were retained by a magnet. MPO was detected in 1:100 diluted serum with limits of detection (LOD) and quantification (LOQ) of 0.18 and 0.62 ng mL<sup>-1</sup>, respectively, in less than 15 min.

**Conclusion:** This work demonstrates that ELFS can be produced entirely using a highly affordable manual screen printing process. Such ELFS have been exploited to simplify and shorten handling of immunomagnetic assays. As a result, MPO was detected at clinically relevant concentrations in diluted human serum, in less than 15 minutes, and with minimal handling by the user. We suggest that ELFS could facilitate production of simple and economical electrochemical immunomagnetic POC devices.

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## Anderson localization to mediate the optomechanical coupling at the nanoscale

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In engineered cavities in optomechanical crystals, fabrication imperfections open extra channels for energy losses, as well as hinder the theoretical optomechanical coupling by limiting energy transfer. Improving state-of-the-art nanofabrication techniques to reduce disorder tends to be the main approach to reduce such losses. Alternatively, deliberately introducing disorder in photonic or phononic nanostructures leads to Anderson localization, where light or elastic waves are efficiently confined due to coherent back-scattering, without requiring any designed cavity. Such randomly localized modes provide a new toolset for phonon-photon interaction.

## In-plane thermal transport by $3\omega$ -Völklein method

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The thermal conductivity ( $\kappa$ ) is an important property of the thermoelectric materials, because the decrease of the  $\kappa$  increases the thermoelectric material efficiency (Figure of Merit). In this context, the ultrathin films present a very low  $\kappa$  and thus to measure the  $\kappa$  during the growing of these films is key for understanding the growth process, besides to obtain ultrathin films with lowest  $\kappa$ . Thus, techniques that can measure the  $\kappa$  of ultrathin films are essential. Among these techniques, the  $3\omega$ -Völklein method stand out for its high sensitivity for measuring the  $\kappa$  in-plane in ultrathin films. In this work, we designed and fabricated a microdevice with  $\text{SiNi}_x$  membrane for  $3\omega$ -Völklein method to characterize the in-plane thermal transport of ultrathin films of a variety of materials, from metallic to polymer. We also show that the high sensitivity of the technique can be used to monitor thin film growth during the early steps of film formation.

# Simple strategies for the functionalization of graphene nanocomposite electrodes with gold and silver nanoparticles

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Electrodes based on nanocomposites can be defined as the result of combining two or more different materials in solid phase where, in which one of them is at nanoscale dimension.<sup>1</sup> In addition, these nanomaterials do not lose their individual identities but still impart their properties to resulting hybrid novel material. Building blocks with dimensions in the nanosize range enable the possibility to develop new materials with unprecedented versatility and improvement in their physical and chemical properties.

Among the wide range of nanocomposites, the development of nanocomposites based on conductive phases dispersed in polymeric matrices has led to important advances in electronics and electrochemistry. In general, nanocomposite materials based on different forms of carbon nanostructures as conductive phase; such as graphite, carbon nanotubes and graphene, have played a leading role in the analytical electrochemistry.

In this communication, we present different strategies for the functionalization of graphene nanocomposite electrodes with noble metal nanoparticles<sup>2</sup> in terms of:

- a) Incorporation of the nanoparticles in the matrix
- b) Direct functionalization of graphite / graphene with nanoparticles

Previous studies proved the feasibility of our experimental procedures for the in-situ modification of different carbon allotropic forms in order to enhance the electrochemical performance when these are integrated into nanocomposite sensors.<sup>3</sup>

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## **Modelling of the current compliance effects in the I-V characteristics of memristors devices**

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A SPICE implementation of a memristor model able to describe the current-voltage loops in bipolar resistive switches including the current compliance effect is reported. In particular, this work addresses the implementation of MIM structures for ReRAM applications by means of SPICE simulations. Specifically, the effect of the current limit is investigated. The model is based on the combination of a diode-like device as the switching element and the logistic hysteron formalism for the memory effect. It is shown how the proposed circuit reproduces the main features of the experimental curves.

## Synthesis of curcuminoid-MOFS using sustainable CO<sub>2</sub> methods. Comparison with solvothermal method

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In the last decades, with the increase of environmental concern and the emergence of green chemistry, the need of new safer and more environmentally friendly processes has raised attention among the scientific community. The substitution of hazard solvents is an important step to achieve this objective.<sup>1</sup> The use of supercritical fluids emerges as an alternative to toxic or pollutant organic solvents. Specifically, supercritical carbon dioxide (scCO<sub>2</sub>) is highly used due to their special properties of non-flammability, negligible toxicity, stability and low critical temperature and relatively low critical pressure.<sup>2,3</sup> In this work, the preparation of hybrid materials formed by the bonding of different curcuminoids, bioactive natural molecules, and metals using supercritical carbon dioxide (scCO<sub>2</sub>) as a solvent is proposed. The results will be compared with the experiments performed using the solvothermal method previously reported for this type of molecules in the literature.<sup>4</sup>

The final purpose of these compounds here is to explore their use as active components in three-terminal electrodes devices (FETs, field effect transistors), working at nanoscale and in case of the achievement of porous materials also their possible use in processes of adsorption/desorption.

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# Fluorescent BODIPY-anionic boron cluster conjugates for cell tracking and neutron capture therapy

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Boron neutron capture therapy (BNCT) is a promising binary therapy for the treatment of cancer, because malignant cells can be selectively targeted and destroyed in the presence of healthy normal cells. A large number of functionalized boron clusters have been designed as boron delivery vehicles. The anions closo-dodecaborate  $[B_{12}H_{12}]^{2-}$  and metallacarboranes  $[M(C_2B_9H_{11})_2]^-$  (M=Co or Fe) possess exceptional chemical and hydrolytic stabilities, uncommon physico-chemical properties in water and low toxicity, making them and their derivatives ideal candidates for BNCT. Research has focused on the development of improved BNCT agents with higher tumor selectivity for being accumulated in tumor cells. An important point is the assessment of the amount of  $^{10}B$  that has reached the target sites, which must be monitored during the in vivo biodistribution. BODIPY-type molecules have found application in imaging, biological labeling and fluorescent probes due to their remarkable high extinction coefficients, low molecular weights, high photochemical stabilities and membrane cell permeability properties.

Therefore, boron clusters-substituted BODIPY dyes could show enhanced permeability and are promising as boron delivery drugs for BNCT. Herein, the design, synthesis, characterization and fluorescence study of a new family of BODIPY derivatives will be presented. Linking the BODIPY to  $[B_{12}H_{12}]^{2-}$  and  $[M(C_2B_9H_{11})_2]^-$  affords fluorescently labelled molecules that allow to know their biodistribution and cellular uptake. The internalization of the dyes inside cells can be monitored through flow cytometry and confocal microscopy analyses.

## **Solidification at the nanoscale. The Guyer-Krumhansl-Stefan problem**

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The heat flux across a nanowire is computed based on the phonon hydrodynamics formalism, i.e., on the Guyer-Krumhansl equation. Slip conditions with a slip length depending on both temperature and size are introduced at the outer boundary. An explicit expression for the effective thermal conductivity is derived and validated against experimental data across a given temperature range, providing excellent agreement. For the validation, we use values obtained recently by a collaborating research group. Both factors yield an improved accuracy of the theoretical predictions with respect to experimental data.

# Thermal properties of novel graphene nanofluids ideal as coolants for computer cooling systems

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Heat transfer fluids have been extensively used from low-temperature applications (like microelectronics cooling) to high-temperature ones (i.e. concentrated solar power). However, their low thermal conductivity is still a limit on performance. One way to enhance thermal properties is to disperse nanomaterials, such as graphene flakes in the base fluid. In this work, we have developed stable graphene nanofluids with enhanced thermal properties, suitable for cooling applications. These nanofluids have a homogeneous composition and are extremely stable over time, which are key factors for a proper thermal characterization and for their final application. In summary, we have i) prepared graphene nanofluids in two base fluids with a higher boiling point than water: dimethylacetamide (DMAc) and dimethylformamide (DMF), ii) modified the 3-omega technique to make it suitable for measuring the thermal conductivity of liquids, and iii) determined the influence of graphene concentration on the nanofluid thermal conductivity, specific heat capacity and speed of sound.

Our results show how a small percentage (0.18%) of graphene in DMAc leads to a substantial improvement (48%) in thermal conductivity, as well as an enhancement of the specific heat capacity (18%) by dispersing 0.11% of graphene in the same fluid. We also observed a progressive increment of the speed of sound as function of graphene concentration.

# Graphene-based electrochemical biosensor for the determination of phenolic compounds

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Graphene is an extraordinary nanomaterial given its chemical and electrochemical properties. The use of graphene as a transducer, both as graphene oxide (GO) or electrochemically reduced graphene oxide (ERGO) forms, may provide enhanced electroactivity for biosensors. Furthermore, it is possible to take advantage of its chemical structure, i.e. it is possible to use remaining carboxylic acid groups after the electrochemical reduction as anchoring points to create covalent bonds with biomolecules. These features make possible the building of improved biosensors.

In this study, it is postulated an enzymatic biosensor from a graphene platform using its chemical properties. Biosensor uses covalent bonds formed with the EDC reaction (N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride), where EDC activate the linkage among graphene carboxylic groups and enzyme amine groups. The used enzyme is laccase, which acts as a catalyst in the oxidation of phenolic compounds.

Phenols are high priority pollutant compounds, present in biological degradation process and in industrial waste. Presence of high concentrations of phenols in food can indicate lack of freshness. Moreover, the extreme toxicities of some of these phenolic compounds make their determination of major concern in environmental analysis.

There are various ways to quantify phenolic compounds. This communication describes an electrochemical biosensor method, which can be an alternative in front of spectrophotometric reactions or heavy instruments as HPLC or HPLC-MS. Biosensor-based methods provide some advantages such as easy and fast operation, low maintenance costs and high sensitivity.

Thus, the goal of this study is to develop biosensors for determination of phenols using laccase enzyme on electrode platforms of ERGO (Enzyme-ERGO-GEC). Catechol calibration curves using different platforms (Enzyme-ERGO-GEC, ERGO-GEC and GEC) are compared and it is observed that graphene enhances sensitivity in front of a bare electrode and also that the signal is improved with the use of the enzyme.

# Growth and Characterization of Transparent Conducting SrVO<sub>3</sub> Thin Films

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Transparent conductors having high electrical conductivity and high optical transparency are of major interest for oxide electronics, particularly for displays and solar panels. So far, tin-doped indium oxide In<sub>2</sub>O<sub>3</sub>:Sn (ITO) has been most widely used as it reaches a good balance between the two above-mentioned features. However, resources of indium are running out. Also, the improvement of the electronic properties of ITO approaches its limit. This awakens the interest for, so called, transition metal oxides, a class of materials that is abundant in nature and can reach higher conductivities.<sup>1,2,3</sup>

Here, we present the growth and characterization of SrVO<sub>3</sub> thin films grown by pulsed laser deposition on (001)-oriented SrTiO<sub>3</sub> and (LaAlO<sub>3</sub>)<sub>0.3</sub>(Sr<sub>2</sub>TaAlO<sub>6</sub>)<sub>0.7</sub> (LSAT) substrates. It is found that textured, single phase and flat films can be obtained at an oxygen partial pressure P<sub>O<sub>2</sub></sub> of 4x10<sup>-7</sup> mbar and in a range of substrate temperatures going from 700 to 800°C. Films grown at higher P<sub>O<sub>2</sub></sub> display, in addition to the main SrVO<sub>3</sub> phase, the presence of spurious phases (identified as Sr<sub>3</sub>V<sub>2</sub>O<sub>8</sub>, etc.) which correlates with an enhanced surface roughness<sup>4</sup> and a higher resistivity. On *in-situ* grown Hall bar devices on LSAT under optimal conditions, we obtain a resistivity of 7.2x10<sup>-5</sup> Ω cm, a carrier density of 2x10<sup>22</sup> cm<sup>-3</sup> and mobility of 4.4 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>. This value of resistivity is close to the state-of-art reported value (2.8x10<sup>-5</sup> Ω cm)<sup>1</sup> and lower than the standard value of ITO (≈ 10<sup>-4</sup> Ω cm).<sup>2,3</sup>

By spectroscopic ellipsometry measurements we observe a plasma energy of 1.2 eV in two samples deposited on LSAT at optimal conditions. This value confirms the transparency of our films in the visible range as the plasma energy is an indicator of the free carrier reflection edge and hence the onset of light absorption and/or transmission. Moreover, in agreement with earlier results,<sup>1</sup> measurements of the transmittance reveal a high transparency over the whole visible spectrum.

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## Different Contributions in Electroresistance of BaTiO<sub>3</sub> Films

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Ferroelectric tunnel junctions (FTJs) have emerged as promising candidates for novel memory devices. Naturally, the success of this approach relies on the ability to build ferroelectric tunnel junctions with large electroresistance (ER) response. In ferroelectric tunnel junctions, ER can be understood on the basis of the change of the tunnel barrier height upon polarization reversal in presence of asymmetric electrodes. In that case the FE switching is expected to be a fast process ( $\ll 1\text{ms}$ ). However, other mechanism may also contribute to the electroresistance, such as space-charge effects or genuine ionic motions. These processes may induce radically different junction's response including longer time responses.

Therefore, investigating the time-dependent response of dynamic of ER in FTJs is crucial to fully understand its origin. Here we report on the systematic investigation of the ferroelectric polarization  $P$  and ER dependence on temperature and writing time of Pt/La<sub>0.5</sub>Sr<sub>0.5</sub>MnO<sub>3</sub>/BaTiO<sub>3</sub>/La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub>/SrTiO<sub>3</sub> Ferroelectric Tunnel Junctions. Our results reveal that the different conductance states of the barrier have a radically different sign, magnitude and dependence on the writing time (even for writing times longer than 1s) depending on sample thickness. Moreover, it is also observed that the temperature dependence of the ER does not follow closely the  $P$  dependence. These observations suggest the observed ER is not solely dictated by the ferroelectric polarization. Therefore, we conclude that ER effect results from a cooperative combination of the FE polarization switching and a slower process, likely: ionic motion, which will be discussed. We believe that the presented results will help to the better understanding of the ER phenomena in both thin and thick ferroelectric films.

## Engineering edge structure and electronic properties of graphene nanoislands

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The possible applications of graphene at the nanoscale require a precise control of its structural and electronic properties. The interfacial interaction between graphene and the underlying substrate can control the morphology and edge atomic structure of the nanostructure, dope the Dirac cones and induce band gaps or spin-polarization.

In this work, we show by using Scanning Tunneling Microscopy and Spectroscopy how this interfacial interaction can be effectively tuned by metal intercalation and used to engineer the properties of graphene nanoislands (GNI). On the catalytic Ni(111) where we grow the GNIs, the strong interaction determines a selection of shape and edge structures. The Dirac cone, strongly affected by the substrate, turns into gapped spin-polarized graphene bands. After intercalation of Au, GNIs are found on top of the Au overlayer or embedded in it. They are chemically and electronically decoupled from the substrate, and their edges present an electronic state possibly polarized in spin.

## Miniaturized multi-sensing platform for pH and dissolved oxygen monitoring in organ-on-a-chip systems

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Organ-on-a-chip (OOC) systems are microfluidic cell culture devices used to simulate tissue or organ level physiology. Their finality is to increase the understanding of the biological processes as well as to develop improved diagnostic and more effective tools for drug screening analysis. Due to the importance of OOC systems, the need for a continuous monitoring of these systems has increased its interest. In this work, a multi-analyte real-time sensing platform printed on plastic substrate is presented. For this purpose, pH and dissolved oxygen (DO) miniaturized electrochemical sensors have been integrated in a small volume chamber for monitoring simultaneously their concentration in the inlets or outlets of the OOC system. The working, counter, and pseudo-reference microelectrodes are printed by inkjet printing technology (IJP). Specifically, the working electrode for the DO sensor has been printed using a gold ink and for the pH sensor with platinum. The pseudo-reference electrodes are printed with silver and the counter with platinum. The three inks are nanoparticle based inks and all of them are commercially available. After the sintering process microelectrodes show excellent conductivity  $1.38 \times 10^7$  S/m for Ag,  $2.08 \times 10^6$  S/m for Pt and  $7.64 \times 10^6$  S/m for Au. Iridium oxide film was electrodeposited as the pH-sensing material and sodium hypochloride was printed on Ag electrode to obtain Ag/AgCl. pH calibration curves show super-Nerstian response (65-70 mV/pH) and DO sensor shows a linear response in the range between 0-8 mg·L<sup>-1</sup> of DO, which demonstrates the good behaviour of the multi-sensing platform.

## **Catechol-based bioinspired adhesives and coatings**

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Inspired by the chemical nature of mussels, catechol-based materials have been studied deeply for their application in underwater and wet environments. In our work, the design of novel polymers containing catechols is presented with the final goal of being applied as tissue adhesive.

## Electrochemical characterization of SWCNTs based microelectrodes fabricated by inkjet-printing

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In this work, the fabrication and characterization of disposable electrodes for electrochemical biosensing using inkjet printing is presented. Inkjet printing is an ideal alternative for prototyping as well as for the heterogeneous integration of different components and materials aiming at the development of flexible and low-cost devices. These electrodes are intended to be used as a platform for the point of care diagnosis of infectious diseases.<sup>1,2</sup> Each electrochemical cell is composed by a working electrode, a counter electrode and a reference electrode printed onto 125 µm flexible substrates of polyethylene terephthalate (PET). The working electrode is printed with a specially designed formulation of SWCNTs ink, whereas the counter electrode is printed with a gold ink and the reference electrode with a commercial silver nanoparticle ink. Here two approaches for the printing of the working electrodes have been used. In the first approach, the electrodes are printed with SWCNTs ink directly over the substrate, while in the other one, in order to improve the conductivity of the electrodes, a gold layer is printed onto the substrate and, on top of it, the electrodes are finally printed with SWCNTs inks. All inks allow their sintering at low-temperature (150 °C) in a short time. In addition, a printable dielectric ink formulation was applied as a passivation layer in the biosensor device. The electrochemical response of the printed electrodes and the integrated platform itself is evaluated by cyclic voltammetry in solutions containing redox species, such as potassium ferricyanide/ferrocyanide or hydroquinone. The results show that inkjet printing electrodes could lead to the development of fully printed electrochemical biosensors.

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## **Fast and simple microwave synthesis of functional multimaterial gold nanoparticles**

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Multi-material nanoparticles exhibiting more than one functional property are interesting because of the potential applications in several fields such as biological tagging, medical diagnostics and treatment, optical and electro-optical applications, batteries improvement, solar energy harvesting and others. We report the microwave synthesis of multi-component nanoparticles composed by gold and metal oxide nanoparticles, comprising superparamagnetic iron oxide NPs (SPIONs) and titanium dioxide NPs (TiO<sub>2</sub>). Structural, compositional and functional results of these synthesis have been characterized through transmission electron microscopy (TEM), scanning electron microscopy (SEM), ultraviolet-visible-near infrared spectroscopy (UV-Vis-NIR), attenuated total reflectance Fourier transformed infrared spectroscopy (ART-FTIR), magnetometry and chemical analysis. This work also aims at the photocatalytic performance evaluation of the Au-TiO<sub>2</sub> NPs to obtain hydrogen from gaseous water/ethanol mixtures.

## **Synthesis of ABO<sub>3</sub> perovskite type nanoparticles**

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A successful methodology for the synthesis of perovskite nanoparticles BaZrO<sub>3</sub>, BaHfO<sub>3</sub> and BaTiO<sub>3</sub> have been achieved by using solvothermal and microwave polyol approach. Triethylene glycol (TREG) is used as capping ligand and providing nanoparticles stable in polar solvents for long time periods.

Perovskite nanocrystals have structural and physical properties that are strongly dependent on size, shape, crystallinity and surface composition and using this new methodology the nanoparticles obtained are highly crystalline (cubic structure for BZO and BHO, and tetragonal in BTO) with uniform size and shape (Cubic-like and spherical).

The influence of different parameters like time, temperature and water content has been studied and a tuning of the nanoparticles size was established. Using the solvothermal approach nanoparticles from 2 to 40nm can be produced with a narrow dispersion.

Nanoparticles, have been characterized by several common physical laboratory techniques: HRTEM, IR, X-Ray Powder Diffraction (XRPD), Malvern zeta sizer. With these techniques, the final size, shape, composition, crystal, showing the high-quality crystals generated.

## Plasmonic metamaterials for opto-mechanical sensing

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Plasmonic near-field interactions are highly sensitive to the distance between neighbouring particles. This principle can be exploited to measure the deformation of elastomeric plasmonic metamaterials for different types of applications. In this work, we study the spectral shift upon deformation of several plasmonic metamaterials based in different kind of close-packed plasmonic nanostructures (i.e. nanodiscs and shells). The plasmonic nanostructures were prepared by different fabrication approaches based on surface nanopatterning, and transferred/embedded into elastomeric substrates (PDMS).

## **Thin film germanium photonic architectures exhibiting enhanced absorption from VIS to NIR frequencies**

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The design of ultrathin semiconducting materials that achieve broadband absorption is a long-sought-after goal of crucial importance for optoelectronic applications. To date, attempts to tackle this problem consisted either on the use of strong – but narrowband – or broader – but moderate – light trapping mechanisms. In this work, we present a strategy that achieves broadband optimal absorption in arbitrarily thin semiconductor materials for all energies above their bandgap. This stems from the strong interplay between Brewster modes, sustained by judiciously nanostructured thin semiconductors on metal films, and photonic crystal modes. We demonstrate broadband near-unity absorption in Ge ultrathin films that extend from the visible to the Ge bandgap in the near infrared and robust against angle of incidence variation. Our strategy follows an easy and scalable fabrication route enabled by soft nanoimprinting lithography, a technique that allows seamless integration in many optoelectronic fabrication procedures.

## **Cross correlation of resistive switching characteristics in memristors devices**

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A statistical analysis of the set and reset parameters extracted from experimental current-voltage (I-V) characteristics of memristive structures were carried out. The obtained results allowed proposing an analytic expression for the different relationships between these parameters with the aim of improving a memristor model. The results provide features for the variability implementation in the model.

## Three-dimensional printing: concept and potential for sensing applications

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With the ever-increasing demand of rapid fabrication of analytical devices, three-dimensional (3D) printing has emerged as an alternative prototyping technology. The potential of this technology to create almost any imaginable geometry has opened a new paradigm in research laboratories. Generally, 3D technology requires two different stages to obtain the final functional scaffold. The first stage is to design the structure using computer aided design software and then the model is sliced in layered information for printing. In the second stage, the most important part is to choose the correct material for the desired application. Some materials have better mechanical properties while others can undergo acid and basic media conditions. Herein, we will describe the different stages, showcase the potential of 3D-printing technology for analytical applications and share our knowhow in the field.

## Engineering bacterial cellulose during the biosynthesis

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Bacterial cellulose (BC), i.e. cellulose produced by bacteria, is a biopolymer with the same molecular formula as the cellulose generated by plants, but with distinct characteristics. It does not contain potential sources of toxicity that are present in plants' cellulose, as lignin and hemicelluloses. Moreover, due to its nanofibers conformation, it exhibits higher transparency, high water holding capacity and hierarchical porosity. Other features are its biodegradability (via enzymatic processes) and chemical and physical tunability.<sup>1,2</sup> Thus, the bacterial cellulose is a promising candidate as green resource for the fabrication of advanced multifunctional materials.

This research presents a strategy to create multifunctional materials using the bacterial cellulose as a platform. Therefore, firstly the porosity and shape of the BC films structure will be studied under different drying conditions. Secondly, a mold-strategy to nanostructure films during the biosynthesis growth will be presented. The aim is to synthesize nanoparticles (metals and metal oxides) in different parts of the cellulosic matrix to create delimited zones with specific characteristics in a same BC film.<sup>3</sup> Finally, this material is expected to show a multifunctionality afforded by the combination of the nanoparticles.

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# Voltage-controlled magnetism in Fe<sub>60</sub>Al<sub>40</sub> (at. %)/(100) PMN-PT multiferroic heterostructures

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Multiferroic heterostructures consisting of 50 nm-thick Fe<sub>60</sub>Al<sub>40</sub> (at. %) films grown by co-sputtering on top of commercially available (100) PMN-PT single crystals (32 mol. % of PT and 0.5 mm-thick) have been synthesized. The Fe<sub>60</sub>Al<sub>40</sub> layers are highly textured along the (110) planes and exhibit ferromagnetism, evidencing that the FeAl alloy grows partially, at least, in an atomically disordered state.<sup>1</sup> The (100) PMN-PT single crystal is a piezoelectric material with a room temperature ferroelectric coercivity of around 2500 V/m (125 V taking into account the thickness of the PMN-PT used).<sup>2</sup> With the aim to investigate the influence of voltage on the magnetic properties, the heterostructures are subjected to a voltage protocol while being measured by vibrating sample magnetometry. Specifically, the piezoelectric is brought to ferroelectric saturation at 200V before registering the hysteresis loop at different negative voltages (i.e., 200 V, 200 V/0 V, 200 V/−20 V, 200 V/−40 V...), resembling the descending branch of the ferroelectric loop. Then, the protocol is reversed (i.e., going from positive to negative saturation and then applying positive voltages in steps of 20 V (200 V/−200 V/0 V, 200 V/−200 V/20 V, 200 V/−200 V/40 V...)). Once the first voltage is applied (i.e., saturation at 200 V), a pronounced decrease in the saturation magnetization is observed. This is ascribed to a partial oxidation of Fe since X-ray diffraction reveals the presence of iron oxide peaks which do not appear in the pristine sample. Upon completion of the voltage protocol, the coercivity, the remanence, the saturation magnetization and the energy product of the hysteresis loops are plotted as a function of applied voltage. The coercivity and remanence monotonically increase with the absolute value of the voltage. However, the descending and ascending dependences are not symmetric, indicating that this behavior might be partially ruled by oxidation and reduction processes since oxygen migration is polarity dependent. Conversely, the saturation magnetization and the energy product exhibit a maximal behavior with peaks between −120 and −160 V and 120 and 160 V for the descending and ascending branches, respectively. Interestingly, the ferroelectric coercivity falls within this voltage range, suggesting that these magnetic properties might be governed by magnetostriction effects in the FeAl layer since the maximum of strain is reached at the ferroelectric coercivity.

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## Epitaxial growth of strontium iridates

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We present a study in thin films growth of complex oxides Strontium Iridates by Sputtering technique. Strontium iridates Ruddlesden-Popper (RP) series ( $\text{Sr}_{n+1}\text{Ir}_n\text{O}_{3n+1}$ ) belong to the 5d perovskites, which exhibit a strong Spin Orbit coupling that can alter the band structure and lead to exotic physical properties. We have achieved to grow epitaxial thin films of the phase  $n=\infty$  ( $\text{SrIrO}_3$ ) and we have studied their properties and stoichiometric dependence on growth conditions (temperature, oxygen pressure and position).

# First-principles computational methods in materials science. SIESTA code integration with AiiDA high-throughput framework for modern computational tasks

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Ab-initio computational techniques are very popular methods of theoretical predictions of novel materials' properties. Modern computational methods allied with high-throughput management systems are aiming at the exascale, allowing materials scientists to describe and analyse thousands of systems containing hundreds of atoms.<sup>1</sup>

My work is mostly devoted calculations of novel 2D-materials' properties. But to achieve the goal of predicting new phenomena in very fashionable systems, one needs also to improve his/her scientific tools. Thus, substantial part of my efforts will be aimed on code development to make frameworks like AiiDA (Automated Interactive Infrastructure and Database for Computational Science) effectively support Siesta computational code. An application in a neighboring field of Computer Science is also possible, if one can effectively control Siesta's input parameters generation and history of preceding calculations - and these are the key features of AiiDA framework.

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## **Multifunctional platform of nanocapsules as drug carrier for angiogenic therapies**

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Cerebral stroke is a leading cause of mortality and disability that affects 15 million people each year worldwide. Our project focuses on developing a novel nanomedicine-based therapy to promote angiogenesis to address neurorepair after stroke. Previous results demonstrated that the factors secreted by endothelial progenitor cells (EPCs-secretome) have therapeutic potential to promote vascular remodeling in the ischemic brain. Compared to the use of EPCs as a cell therapy or the encapsulation of a single growth factor, i.e., VEGF, the encapsulation and controlled delivery of EPCs-secretome as therapeutic agent is clinically interesting in terms of efficiency and safety. In this context, our aim is to take advantage of a nanotechnology approach to achieve the delivery and accumulation of EPCs-secretome in the peri-infracted brain area to promote neurorepair. Specifically, we have engineered a multifunctional polymer nanocapsule platform to encapsulate the EPCs-secretome. This drug delivery system combines the treatment strategy with several diagnostic capabilities. Biodegradable and biocompatible poly(lactic-co-glycolic acid) (PLGA) nanocapsules are synthesized by a double emulsion-solvent evaporation method. PLGA could be further co-polymerized with PEG (to increase the stealth nature of the capsules) and with an intrinsic fluorescent polymer (to in vivo track the particles by fluorescence). Further functionalization is achieved by adding magnetic nanoparticles to the organic phase during the synthesis (to magnetically accumulate the capsules in the area of interest with a magnetic field and track them by MRI). Finally, the synthesis method can be modified to attach PET sensitive radiolabels. The presentation will highlight our recent advances in the development of these multifunctional polymeric nanocapsules and their use for neurorepair after stroke.