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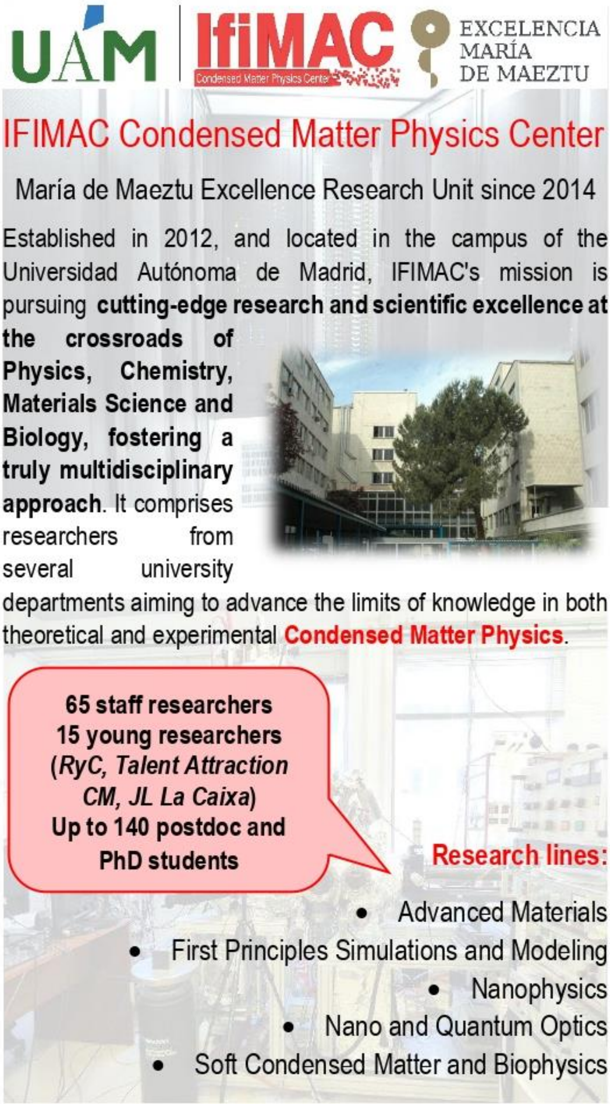

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María de Maeztu Excellence Research Unit since 2014

Established in 2012, and located in the campus of the Universidad Autónoma de Madrid, IFIMAC's mission is pursuing **cutting-edge research and scientific excellence at the crossroads of Physics, Chemistry, Materials Science and Biology, fostering a truly multidisciplinary approach**. It comprises researchers from several university departments aiming to advance the limits of knowledge in both theoretical and experimental **Condensed Matter Physics**.

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May 17 - 20, 2022 • Madrid (Spain)

Consolidated as a reference meeting of Nanoscience and Nanotechnology (N&N) in Spain, the NanoSpain2022 conference is not limited to a conventional presentation of ideas or results, but seeks to deepen the common themes among the participants, also serving as a link between industry and researchers. Over the past years, NanoSpain conference became more and more multidisciplinary and 2022 won't be an exception; covering a broad range of current research in Nanoscience and Nanotechnology.

Since 2004, year the event was launched, NanoSpain conference series aims to agglutinate and coordinate the efforts made in the field of Nanoscience & Nanotechnology by Spanish groups from universities, research institutes and companies.

NanoSpain2022 will offer a multitude of renowned international Keynote and Invited speakers, contributed talks, posters and a commercial exhibition.

We would like to thank all participants, speakers, sponsors and exhibitors that joined us this year. Finally, thanks must be directed to the staff of all organizing Institutions making this event a reality.

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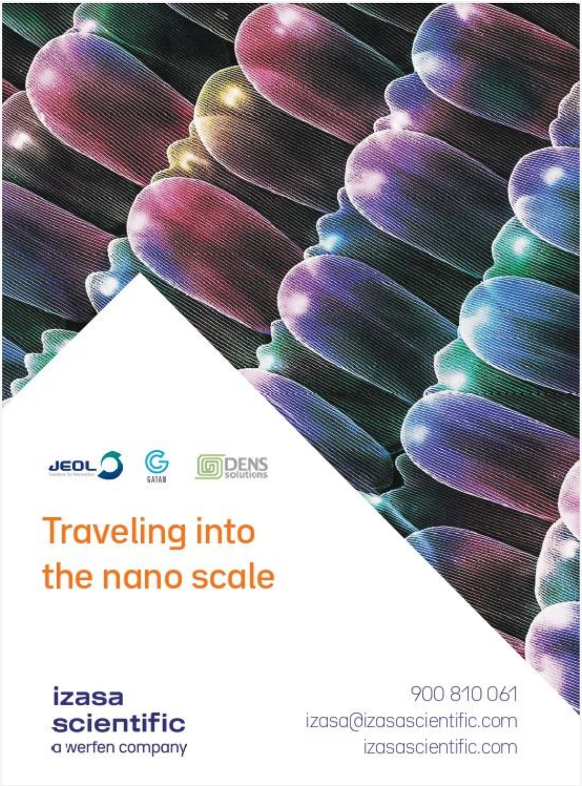

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AGENDA & LOCATION

Tuesday – May 17	**Room**	**Time**
Registration	Main Entrance	08:00-08:45
Opening Ceremony	Auditorium	08:45-09:00
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Poster Session I	Sala de Máquina	14:30-15:00
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Cocktail Lunch (offered by the organisers) Poster session - Exhibition	Sala de Máquina	13:35-14:30

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Exhibition & Poster Sessions	Sala de Máquina	-
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PARALLEL SESSION (PhD Students) - TRACK A Graphene, Nanomagnetism, NEMS/MEMS	Auditorium	14:30-16:00
PARALLEL SESSION (PhD Students) - TRACK B NanoBiotechnology, Simulation at the nanoscale, SPM	Room C	14:30-16:00
NanoSpain2022 Plenary Session	Auditorium	16:45-19:00
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Cocktail Lunch (offered by the organizers). Poster Session - Exhibition	Sala de Máquina	13:00-14:00

Friday – May 20	**Room**	**Time**
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PARALLEL SESSION (PhD Students) - TRACK C SPM, nanophotonics	Auditorium	12:30-13:20
PARALLEL SESSION (PhD Students) - TRACK D Nanomaterials	Room C	12:30-13:10
NanoSpain2022 Plenary Session	Auditorium	14:30-16:30
Exhibition & Poster Sessions	Sala de Máquina	-
NanoSpain2022 Closing remarks	Auditorium	16:30

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GENERAL INFO

FREE WIFI	Ask for details at registration desks
EXHIBITION & POSTER AREA	Sala de Máquina
COFFEE BREAKS	Check the program online for timetables Location: Sala de Máquina
COCKTAIL LUNCH	Offered by NanoSpain2022 organisers Tuesday May 17, 13:35-14:30 Thursday May 19, 13:00-14:00 Location: Exhibition & Poster Area
CONFERENCE DINNER*	Wednesday May 18, 21:00 Restaurant Panamera C/ Fernández de la Hoz, 57 28003 Madrid

*Conference dinner NOT included in Exhibition pass. If you wish to attend, contact the organisers at the registration desk.

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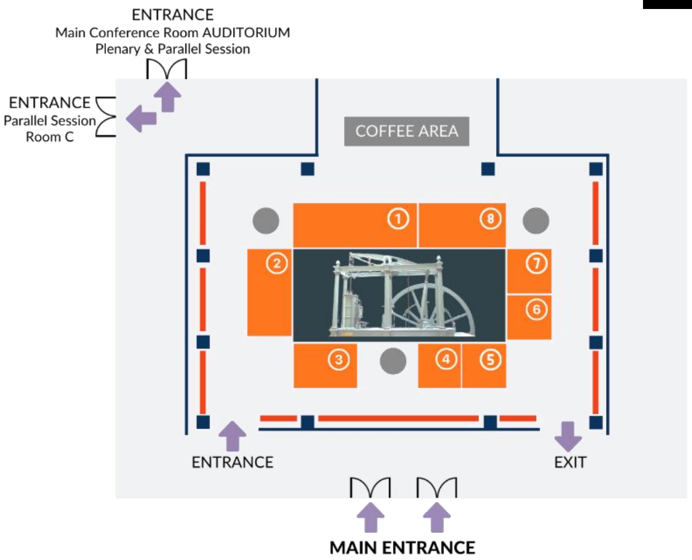

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KEYNOTE SPEAKERS

Cationic Polymeric Nanoparticles for Biomedical Applications

María Rosa Aguilar, Eva Espinosa-Cano, Julio San Román

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Chronic inflammation diseases are ranked as the first cause of morbidity and mortality worldwide. They also cause long-term suffering, disability reduction on the quality of life and high cost to the society. Actual anti-inflammatory drugs present a limited effectiveness due to their hydrophobicity, low bioavailability, and lack of specific targeting. Moreover, anti-inflammatory treatments have associated several side effects limiting their safe use in the clinic. Our group has dedicated great efforts to the preparation of more efficient derivatives of these drugs: drug conjugates [1], drug combinations showing synergistic effects [2] and nanometric drug delivery systems (NDDS) [3].

In this presentation the application of polymer nanoparticles as drug delivery systems for the treatment of inflammatory diseases will be presented. In particular, non-steroidal anti-inflammatory drugs, NSAID (*i.e.* naproxen or ketoprofen) were chemically modified and the methacrylic derivative of the correspondent NSAID was prepared (*i.e.* HNAP or HKT, respectively). These synthetic monomers were used for the synthesis of polymer drugs with a pseudo-gradient microstructure by free radical copolymerization with 1-vinylimidazole (VI). These amphiphilic pseudo-block copolymers self-assembled in aqueous media by nanoprecipitation forming nanoparticles with spherical shape, nanometric size (between 100 and 200 nm) and positive surface charge. These physico-chemical properties demonstrated non-toxicity and a fast sequestration by macrophages which favors accumulation and retention at inflamed areas.

These **cationic anti-inflammatory NPs** have not only been studied as DDS [2,3], but also have been immobilized on surfaces by layer-by-layer (LbL) methodology [4] to avoid foreign body reaction, have been coated with hyaluronic acid in order to achieve active targeting toward CD44 receptor (overexpressed in M1 pro-inflammatory macrophages and cancer stem cells) [5], have been incorporated in self-assembling gels to obtain scaffolds with anti-inflammatory properties and have been used as genetic vetors.

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[5] Eva Espinosa-Cano, Miguel Huerta-Madronal, Patricia Camara-Sánchez et al. *Materials Science & Engineering C* 2021, **124**: 112024

A closer look at graphene bandgap engineering

[1]**Peter Bøggild,** [1]Lene Gammelgaard, [1]Dorte Danielsen, [1]Mads Brandbyge, [1]Anton Lyksborg-Andersen, [1]Tim Booth, [1]A-P. Jauho, [2]Morten R. Thomsen, [2]Thomas G. Pedersen, [1,3]J. M. Caridad, [4]Alfred Jones, [4]Søren Ulstrup, [5]Bjarke S. Jessen, [5]Cory R. Dean, [6]K. Watanabe, [6]T. Taniguchi

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After the initial excitement about graphene's high performant and scientifically rich electronic properties, one of the most obnoxious challenges have been to pattern graphene on a small scale. In theory, nanostructuring of graphene opens for the electronic and photonic properties to be "programmed" to match specific applications or to bring out entirely new physics. In practice, even low levels of edge disorder and contamination associated with even the best lithographic processes, strongly impair the electronic properties. I will discuss our progress in creating lithographic "nanoporous" graphene [1], where we combine encapsulation in hexagonal boron nitride (hBN), high-density lithography, and carefully tuned anisotropic etching process, to pattern graphene on the 10 nm scale, and still preserve the detailed magnetotransport signatures predicted by tight-binding calculations (Fig. 1). The surprising survival of the subtle moire-superlattice signatures associated with twisting of the crystalline interlayers opens for construction of circuits and components that exploit this emerging branch of solid-state physics. I will explain how anisotropic etching of hBN using SF_6, can be used for super-resolution nanolithography, enabling downsizing of features way below conventional lithography limits [2]. Recent nano-ARPES mapping of the bandstructure performed insitu on patterned, gatable devices, confirm that the electric behavior can indeed be explained by a antidot-lattice induced bandgap [3], as predicted 14 years ago [4].

References

[1] B. S. Jessen, L. Gammelgaard, M. R. Thomsen, D. M. A. Mackenzie, J. D. Thomsen, J. M. Caridad, E. Duegaard, K. Watanabe, T. Taniguchi, T. J. Booth, T. G. Pedersen, A-P. Jauho, P. Bøggild, Nature Nanotechnology, 14, 340-346 (2019)

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Figures

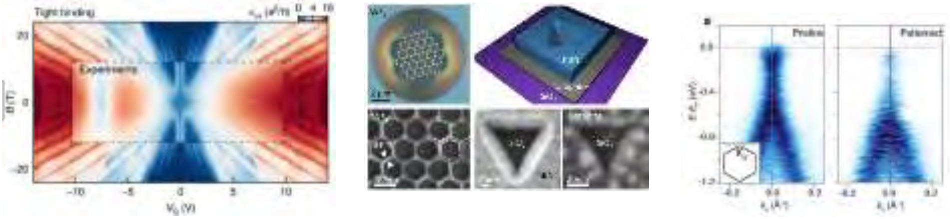

Fig. 1. (Left) Experimental vs theoretical magnetotransport of nanopatterned graphene. (Center) Ultradense patterning using anisotropic etching. (Right) Nano-ARPES of nanopatterned graphene.

Integrating van der Waals materials on paper-electronics

Andres Castellanos-Gomez

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A big chunk of the price tag of electronic components is due to the cost of silicon wafer substrates. Although silicon is a highly abundant and cheap element, the transformation and processing from the raw material into high quality silicon wafers results very costly. In fact, the cost of silicon substrates constitutes ~1/3rd of the total cost of a memory chip and about ~1/10th of the cost of a high-end state of the art micro-processor. The societal, industrial and technological demands of ultra-low-cost electronic components has spurred the quests towards lower cost substrates. This has motivated a surge of works on paper-based electronics in the last years. In fact, paper substrates cost (~0.1 €/m2) is orders of magnitude lower than that of polymer substrates (PET ~2 €/m2 and PI ~30 €/m2) and crystalline silicon (~1000 €/m2).

Despite the promises of paper-based electronics, there are several challenges to be solved. One of the major challenges is that the rough, fiber-based structure of paper makes it impossible to fabricate devices using conventional lithographic techniques. In this talk I will discuss our last works to integrate different van der Waals materials onto standard paper substrates [1-4].

References

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[3] M Lee et al. Nanoscale (2020) 12 (43), 22091-22096
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Figures

Figure 1: Picture of several paper-electronic devices fabricated by integrating different van der Waals semiconductors on standard copy paper substrates.

High-power laser interactions with structured materials and applications

Mattia Cipriani

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The study of the interaction of high-power lasers with structured materials is at present a very active field of research, with a rich physics and a wide range of applications. The use of nano-structured materials in experiments with ultrashort laser pulses, with a time duration in the femtosecond range, allowed to enhance the number of accelerated particles and their energy compared to more usual materials, such as metallic foils [1–3]. On the other hand, the interaction of high-power laser pulses in the nanosecond range with micro-structured materials is being studied for its applications to inertial confinement, for their ability to smooth the beam profile, reduce the parametric and hydrodynamic instabilities and increase laser absorption [4–6]. Finally, the use of micro-structured materials with a combination of nanosecond and picosecond laser pulses allowed to enhance the acceleration efficiency of electrons and ions [7]. The broad interest in these topics recently led to the creation of a dedicated Expert Group by Laserlab-Europe AISBL.
In this talk I will give an overview over recent achievements in the study of the physics of the interaction of high-power laser pulses from the femtosecond to the nanosecond regime with nano- and micro-structured materials highlighting their peculiar features. I will then describe the recent activity of the group of the ABC facility at the ENEA Research Center in Frascati on the interaction of high-power nanosecond lasers with micro-structured materials of low-Z elements.

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Porous silicon, a biodegradable semiconductor for nanomedicine

Frédérique Cunin[a], Sofia Dominguez-Gil [a], Christophe Nguyen [b], Eduardo Cueto-Diaz [a], Arnaud Chaix [a], Magali Gary-Bobo [b], Alain Morère [b], Marcel Garcia [b], Anthony Delalande[c], Chantal Pichon[c], Patrick Midoux[c], Marie Maynadier [d], Jean-Olivier Durand [a]

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The application of nanotechnologies into medicine promises to offer solutions when applied to health challenges such as cancer. Our research projects aim to develop biodegradable multifunctional anti-cancer materials based on mesoporous silicon-based nanostructures to be used for the local treatment of tumors. Porous silicon nanoparticles are fully bioresorbable, and nontoxic *in vivo*, in addition they can be excited by near infrared two photon excitation light offering possibilities for phototherapies, and for light triggered and focalized treatment.

The development of photoactive porous silicon nanovectors functionalized with organic ligands for applications in imaging, photo-activated therapies, as well as for tissue engineering will be presented.

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Electronic excitations and energy dissipation of atoms and molecules approaching metallic surfaces

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Basic understanding of the complex physical and chemical processes that take place at the interface between gas and solids is essential to advance in the mastering and optimization of many technologies and industrial applications. Surfaces are collectors of energy via reception of electromagnetic radiation, heat, and chemical energy. Surface modification can transform the functionality of a system and thus its use. Surfaces can be active agents for atoms and molecules and help to break and create chemical bonds. Although first-principles calculations have very much helped to advance in the quantitative study of static properties, visualizing the time evolution of surface processes at the atomic and molecular level is still a tough task. The adiabatic approximation, in which electronic dissipative effects are neglected, describes reasonably well the dynamics of some of these processes. However, atoms and molecules can generate low energy electronic excitations in metal surfaces even at thermal energies. Therefore, dynamical simulations of these systems should in principle incorporate electronic non-adiabatic effects, in order to analyze how they can affect the outcome of gas-surface reactions.

Quite often, the effect of low-energy electron-hole pair excitations can be included in the theoretical description of the dynamics through an electronic friction coefficient [1]. A widely used model to calculate this friction coefficient is the local density friction approximation (LDFA) [2], which can be directly applied to perform ab initio molecular dynamics with electronic friction (AIMDEF). In this talk, I will provide the theoretical basis of the LDFA and show how it can be applied to improve over adiabatic results based on first-principles calculations. The accuracy of the LDFA approximation will be also tested by comparing its predictions with those of a non-perturbative method, namely time-dependent density functional theory (TDDFT). A jellium cluster will be used as a model system for this purpose [3]. A detailed comparison of the LDFA results and the TDDFT results at the cluster surface, a region in which the electronic density is rapidly varying, shows that a local friction approximation provides a satisfactory enough description of the force linked to the excitation of electron-hole pairs. Thus, the LDFA can be described as an efficient framework to calculate the friction coefficient introduced in multidimensional molecular dynamics simulations.

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Scattering of classical and quantum states of light with angular momentum by dielectric micro/nanoresonators

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The angular momentum of photons[1] affects the interaction between a beam of light and a dielectric particle acting as an optical micro/nanoresonator, which introduces new possibilities to manipulate optical information (encoded in the angular momentum) at very small scales and to gain information about the particle. In this contribution, we discuss some of these possibilities for illumination with classical and quantum states of light.

We consider as resonators dielectric spherical particles of radius ≈250nm-5µm illuminated by light with zero total angular momentum but with spin angular momentum [2]. The projection of the latter into the direction of propagation of the beam gives the helicity Λ. We first study theoretically and experimentally the backscattering of a classical beam with Λ=1 by a micrometer-sized particle. The strength of the backscattering shows a complex and fast dependency on the frequency of the illumination laser. This complex behaviour can be explained by decomposing the backscattered light into the components with helicity Λ=1 and Λ=-1. We show that the Λ=-1 component exhibits spectrally-fast oscillations that are induced by interferences between the multiplicity of higher order modes of the nanoresonator. Theoretical calculations using Mie's theory are in very good agreement with the experimental results. Further, we discuss how the observed response introduces a new tool to characterize the spherical resonators, as indicated by a simple analytical equation that connects the periodicity of the oscillations with the size and dielectric constant of the spherical nanoparticle.

We then consider pulsed illumination of spherical nanoresonators of radius ≈250nm by the two-photon entangled state $|\Psi_+^i> = \phi\,[|+>|+> + |->|->]$, where ϕ defines the envelop and frequency of the incident pulse and $|+>$ and $|->$ corresponds to one-photon states of helicity Λ=1 and Λ=-1, respectively. Due to the spherical symmetry of the nanoresonator, the scattered radiation can be decomposed into two well-defined output states which, for quantum information purposes, should retain a high degree of purity. Recent experiments, however, indicate that this is not always the case [3]. We analyse the loss of purity induced by the scattering process and show that it can be neglibible for adequately chosen conditions. However, it can also become significant when the illumination excites two (or more) spectrally-narrow optical resonances of the nanoresonator. We explain this result by a simple analytical model that shows that the frequency-dependence of the optical response induces a time delay and a frequency shift between the two output states, which results in the undesired loss of purity. Minimizing this effect when engineering the optical response of the nanoresonators is important for quantum information applications.

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Nanocolumnar films: sustainable manufacturing and applications in medicine, energy and aerospace industry

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In this talk, I will briefly show that nanocolumnar films can be manufactured by magnetron sputtering using the glancing angle deposition configuration. This technique is environmentally friendly, since it is carried out at room temperature in a single step and does not involve chemical products (i.e. no recycling issues). Depending on several parameters (mainly the gas pressure, see Fig. 1, the angle of inclination of the substrate and its possible rotation), the nanocolumnar structure can be controlled [1-3]. Furthermore, this method can be scaled up to large surfaces, representing a valid approach for the industrial production of nanostructured films [4]. Then, in the second part of the talk, I will show several applications of these nanocolumnar films in medicine, energy & environment and the aerospace industry, in particular as:
-antibacterial coatings for orthopedic implants [4,5];
-bioelectrodes for an electric stimulation platform *in vitro* [6];
-substrates for the identification of biomolecules in surface enhanced Raman spectroscopy, SERS [7];
-black metal coatings in the visible range [3];
-nanostructured layer for advanced perovskite solar cells [8];
-nanostructured surfaces with photo-induced self-cleaning activity [9];
-magnetic nanopillars [10];
-anti-multipactor coatings for the space industry [11].

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Figure

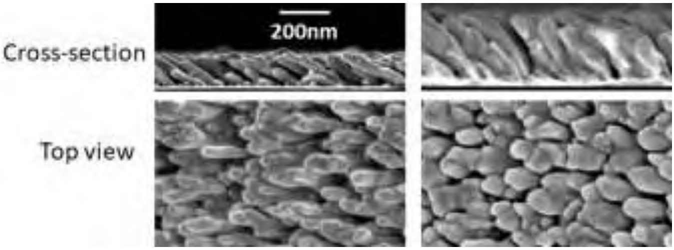

Figure 1: SEM images of Au nanocolumnars films prepared with different pressure: 1.5×10^{-3} (left) and 10^{-2} (right) mbar.

Quantum links between quantum computers

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We have proposed [1] a realistic setup, inspired by already existing experiments [2], within which we develop a general formalism for the implementation of distributed quantum gates. Mediated by a quantum link that establishes a bidirectional quantum channel between distant nodes, our proposal works both for inter- and intra-node communication and handles scenarios ranging from the few to the many modes limit of the quantum link. We can design fast and reliable state transfer protocols in every regime of operation, which, together with a detailed description of the scattering process, allows us to engineer two sets of deterministic universal distributed quantum gates. Gates whose implementation in quantum networks does not need entanglement distribution nor measurements. By employing a realistic description of the physical setup, we identify the most relevant imperfections in the quantum links as well as optimal points of operation with resulting infidelities of $1 - F \approx 10^{-2} - 10^{-3}$.

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Figures

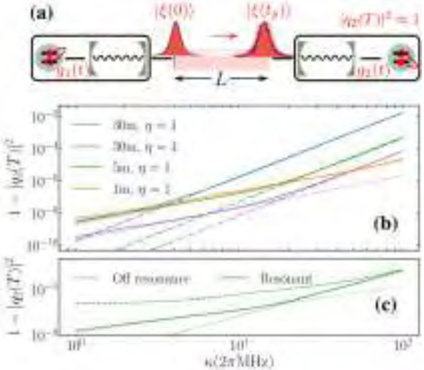

Figure 1: Quantum state transfer between two interlinked quantum computers. (b) Infidelity of the process for commercial waveguides of different lengths. (c) Infidelity in the limit in which free spectral range is too long to formally define traditional controls.

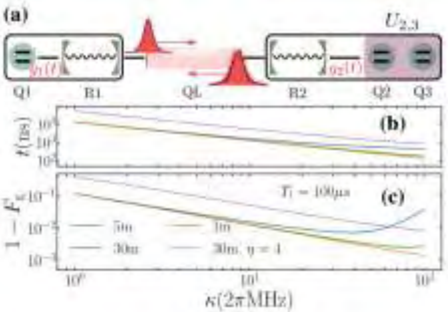

Figure 2: Deterministic quantum gate between two interlinked quantum computers. (a) Duration of the gate for different separations, and (b) infidelity of the gate for qubit with losses.

Nanostructured materials under irradiation: their capabilities as plasma facing materials in fusion reactors

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Nuclear fusion is a promising option for providing clean energy with high-power density and reliable power supply. There are two main approaches to fusion energy: magnetic confinement fusion (MCF) and inertial confinement fusion (ICF). Both of them have recently achieved important milestones, showing that we are on the right path to make fusion energy a reality. However, there are still some challenges which need to be addressed before going to commercial power plants. One of them is the development of plasma facing materials being able to withstand the harsh conditions taking place in these reactors (large thermal loads and radiation fluxes) [1].

So far, coarse-grained tungsten (CGW) is considered one of the most promising candidates as PFM in future fusion reactors since it fulfills most of the highly demanding requirements. However, it has important drawbacks, such as its ability to retain and to interact with light atomic species easily, mainly hydrogen and helium, which leads, among other fatal effects, to: fuzz formation [2], sputtering of the PFM surface, as well as surface blistering, cracking, and exfoliation [3]. Moreover, in the case of MCF, sputtering will additionally affect the energy confinement efficiency by introducing radiative losses which can result in interruption of the reactor operation. Therefore, there is a need to identify alternative materials with better radiation resistance than CGW.

Nanostructurization of W by introducing a large density of grain boundaries (GBs) and/or by producing engineered surfaces with a large surface area, such as needles and foams, have been shown to improve radiation resistance [4–9].

In this talk, based on experimental and multiscale computer simulation data, we will discuss the effectiveness of grain boundaries and free surfaces to release H and He atoms. We will also show the influence of surface finishing on the sputtering yield for W nanoneedles irradiated with low energy ions.

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What makes a catalyst active? Insights from IR nanospectroscopy measurements on single nanoparticles

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The development of optimized (electro)catalysts that can address the grand energy challenges of the 21st century requires in depth understanding of the basic elements that direct the reactivity of catalytic nanoparticles. In this talk I will demonstrate that structure-reactivity correlations within single catalytic nanoparticles can be identified by conducting Infrared nanospectroscopy measurements, while using N-heterocyclic carbene molecules as probes for surface-induced reactivity.[1-3] Using this approach, we detected the influence of different surface sites on the catalytic reactivity of Au and Pt particles and the ways by which site-dependent reactivity and selectivity varies in response to reaction conditions. In addition, by conducting Infrared nanospectroscopy measurements we uncovered the influence of communication between neighboring surface sites on the nanoscale and globular reactivity pattern [4]. These findings provide fundamental understating about the elements that direct the catalytic reactivity of metallic nanoparticles to offer guidelines for the design of optimized catalysts.

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Figures

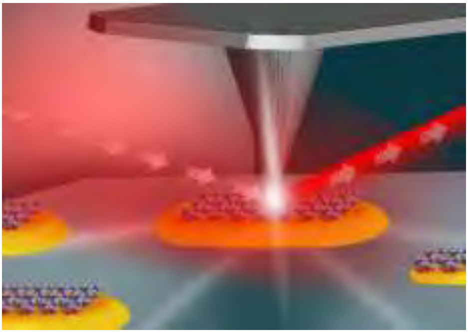

Figure 1: High spatial resolution mapping of catalytic reactivity on the surface of single nanoparticles was achieved by probing the chemical signature of reactant molecules using tip-enhanced IR nanospectroscopy measurements.

Advances in Ultrafast Pulse Laser Irradiation of Metal Nanoparticles

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The vast majority of the applications of metal nanoparticles developed during the last two decades have arisen from their unique optical properties.[1] Within this context, rational synthesis and assembly of metal nanoparticles have been the main research focus, aiming at the design of nanoplasmonic devices with tailored optical functionalities. The progress made in this field is thus to be ascribed to the understanding of the origin of the interaction between light and such nanostructures, the dynamics of which have been thoroughly investigated with significant contributions from short and ultrashort pulse laser technologies.[2]

This presentation focuses on the potential of pulse lasers to provide new fundamental insights into the electron dynamics involved in the interaction of light with the free conduction electrons of metal nanoparticles, that is, localized surface plasmon resonances (LSPRs). The excitation of LSPRs with a femtosecond pulse laser is followed by thermalization of the metal nanoparticle electrons and the subsequent relaxation of the nanocrystal lattice and the surrounding environment, which generally results in surface melting.[3] By contrast, nanosecond irradiation usually induces metal nanoparticle fragmentation and uncontrolled melting due to overlapping excitation and relaxation phenomena. These concepts have been exploited toward the preparation of highly monodisperse metal nanoparticles via femtosecond pulse laser irradiation of polydisperse colloids, or in the fabrication of hollow and alloyed metal nanoparticles.[4]

In addition, pulse laser irradiation has been proven a unique tool for the controlled assembly and welding of colloidal metal nanoparticles by electromagnetic field enhancement at the hot spots of assembled metal nanoparticles.[5] The combination of such gold nanostructures with pulse lasers promises significant chemical and biochemical advances, including the structural determination of organic reaction intermediates, the investigation of phase transitions in inorganic nanomaterials at mild reaction conditions, or the efficient photothermal destruction of cancer cells avoiding damage of surrounding tissue.

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Atomistic Studies of Thermal Transport at the Nanoscale

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Gining control over heat flow at the nanoscale poses a major challenge to current technologies. The issue is not only the reduction of heat dissipation in nanoelectronic devices or the blocking of thermal transport to increase the thermoelectric efficiency, but also to engineer thermal devices to exploit the richness of nanoscale material properties. Thus, analogs of electronic devices, such as thermal rectifiers and thermal transistors have already been proposed. In this context, atomistic design strategies for nanodevices and nanomaterials are required, in particular the combination of computationally efficient atomistic methodologies with quantum transport based approaches. I will address two main topics: (i) Phonon filtering in nanoscale heterogeneous molecular junctions, consisting of molecular wires bridging two different nanocontacts. The obtained spectral phonon gaps are shown to strongly correlate with the properties of the vibrational spectrum of the specific molecular species in the junction. The filtering effect results from a delicate interplay between intrinsic vibrational structure of the molecular chains and the different Debye cutoffs of the thermal baths; (ii) A nanoscale phononic analog of the Ranque-Hilsch vortex tube in which heat flowing at a given temperature is split into two different streams going to the two ends of the device, inducing a temperature asymmetry. The nanoscale prototype consists of two carbon nanotubes (capped and open) connected by molecular chains. Our results show that the structural asymmetry in the contact regions is the key factor for producing the flux asymmetry and, hence, the induced temperature-bias effect.

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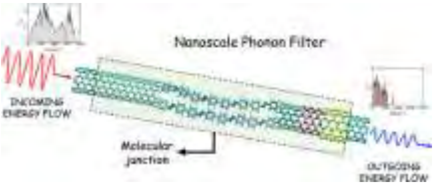

Figure 1: Schematic representation of the molecule-based nanoscale phonon filter.

White Light Emission from Low Dimensionality Halide Perovskites

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Hybrid halide perovskites are a novel class of semiconductor materials with promising and versatile optoelectronic properties, enabled by their chemically adjustable structures and dimensionality. The diversity in the metal ions, halide anions, and organic spacers enables a wide range of materials with highly tunable properties and variable dimensionalities. These materials are studied for various applications such as solar cells, detectors, and light-emitting diodes. The ability to control and adjust the optical properties for a required application is significant. Thus, an improved understanding of the structure and optical mechanisms is crucial.

Specific low-dimensionality hybrid halide perovskites exhibit white-light emission at room temperature, associated with self-trapped excitons (STE), making them ideal candidates for illumination applications. We study the correlation between structural motifs of low dimensionality (2D, 1D) halide perovskites and their STE emission. We further study how the composition and specifically exchanging the halide anions while maintaining the structure affect the STE properties.

Figure

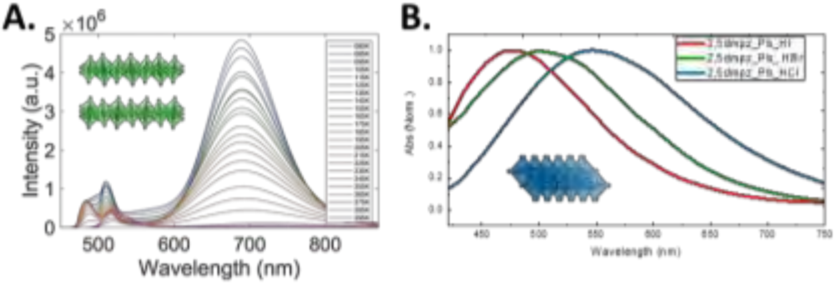

Figure 1: A. Temperature dependent photoluminescence of BA_2PbI_4 2D perovskite exhibiting transition from narrow photolumineseence at room temperature to STE emission at low temperatures. B. STE emission of 1D perovskite – (2,5dmpz)PbX_4 (X = Cl, Br, I).

Multimodal nanotracers for molecular imaging of cardiovascular diseases

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Iron oxide nanoparticles are the eternal promise in the field of diagnosis by non invasive molecular imaging. These nanomaterials have some remarkable properties to fulfil such promise: biocompatibility, flexible surface chemistry and tailored synthesis. However, traditional superparamagnetic iron oxide nanoparticles, active as “negative” contrast probe in magnetic resonance imaging, are not suitable for many diseases. The identification of nanoparticle uptake in the area of interest is many times imposible because of the dark, hypointense, signal these nanoparticles provide.

^{68}Ga nanoradiomaterials (^{68}GaNRM) join both aspects: biocompatible nanoparticles with tailored properties providing hot-spot (bright) signal simultaneously in magnetic resonance imaging and positron emission tomography.[1] In our goup we are using these nanomaterials for the unambiguos detection of different molecular aspects of cardiovascular diseases, such as inflammation,[2] thrombobitc events[3] and, particularly, atherosclerosis plaque development.[4–6]

This talk will focus on the advantages of using such NRM as molecular imaging probes, their combination with other strategies (particularly the use of bioorthogonal chemistry) and possibilities for clinical translation.

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Hybrid materials for 3D cell model fabrication

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3D-printed cell models are currently in the spotlight of medical research.[1] Whilst significant advances have been made, more realistic models that can mimic the different physical forces and stress factors that cells experience in healthy and pathphysiological conditions are still needed.[2] One method to achieve these properties is via hybrid biomaterials, in which inorganic nanoparticles (NPs) and organic materials can be combined to produce a biocompatible and stimuli-responsive environment.[3,4] The NPs can provide the physical properties of interest (i.e. optical response, heating, magnetic response, or mechanical strength, etc.), while the organic matrix (polymers, proteins, etc.) can provide the structural microenvironment for cell growth, with controlled porosity or responsiveness toward external stimuli.

In this context, we have been focussed on the synthesis of hybrid inks, composed of plasmonic gold NPs (AuNPs) and functional polymers, which can be printed using high resolution 3D printing techniques. Spatial resolution can be controlled on the micro-scale, allowing multiple different inks to be deposited within proximity. This technique can be used to print human cells combined with the stimuli responsive inks, thereby generating different models of pathological interest. For example, we are interested in generating a model of the arterial wall, composed of 3D printed endothelial and smooth muscle cells. By combining those living inks with a stimuli-responsive hybrid ink, which can contract and expand in response to externally applied light in resonance with the localized surface plasmons of incorporated AuNPs, we aim to simulate the physical changes in the arterial wall. Additionally we are exploring the use of 3D-printed scaffolds containing AuNPs to study tumor growth.[5] This model aims to allow the analysis of relevant cancer biomarkers in situ, thanks to the sensing properties of the AuNPs which can be used as Surface Enhanced Raman Scattering (SERS) substrates for Raman-active molecules.

These sophisticated models not only require improvements in cell engineering techniques and in the development of new hybrid materials, but also advanced imaging tools to accurately characterize them.[6] As such, we are exploring methods to improve imaging resolution and speed, taking advantage of the inherant NPs of each model to act as contrast agents for correlative imaging techniques.[7]

All these aspects will be highlighted to discuss how our advanced hybrid materials could be used in biomedical applications and the advantages they offer over current materials and techniques.

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Nanoactuators for Therapy and Diagnosis

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In the last decades, inorganic nanoparticles have been steadily gaining more attention from scientists from a wide variety of fields such as material science, engineering, physics, or chemistry. The very different properties compared to that of the respective bulk, and thus intriguing characteristics of materials in the nanometre scale, have driven nanoscience to be the centre of many basic and applied research topics. Moreover, a wide variety of recently developed methodologies for their surface functionalization provide these materials with very specific properties such as drug delivery and circulating cancer biomarkers detection. In this talk we describe the synthesis and functionalization of magnetic and gold nanoparticles as therapeutic and diagnosis tools against cancer.

Gold nanoprisms (NPRs) have been functionalized with PEG, glucose, cell penetrating peptides, antibodies and/or fluorescent dyes, aiming to enhance NPRs stability, cellular uptake, and imaging capabilities, respectively. Cellular uptake and impact were assayed by a multiparametric investigation on the impact of surface modified NPRs on mice and human primary and transform cell lines. Under NIR illumination, these nanoprobes can cause apoptosis. Moreover, these nanoparticles have also been used for optoacoustic imaging, as well as for tumoral marker detection using a novel type of thermal ELISA and LFIA nanobiosensor using a thermosensitive support.

Exploring the Zoo of Layered Quantum Materials

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Abstract

There has been a recent rush of predictions of a variety of astonishing phenomena and functionalities that can be discovered in layered quantum materials, from topological superconductivity or disipationless conductivity at the boundaries of 2D topological insulators, to emergent particles with fractional charge and statistics or exotic collective behaviours that arise from strong interactions.

A suitable combination of experimental techniques: STM/STS, Helium Atom Scattering and spin-resolved ARPES will be used to characterize the properties of both single crystals, such as a type-II Dirac semimetal (1T-$PtTe_2$(100) [1]), a predicted topological superconductor (1T-$PdTe_2$(100) [2]) or an antiferromagnetic Topological Insulator ($MnBi_2Te_4$ (001) [3]) and epitaxial monolayers, such as 2D topological semiconductors (2H-$MoTe_2$/gr/ Ir(111)) or Quantum Spin Hall Insulators (1T-$MoTe_2$/gr/ Ir(111) [4]).

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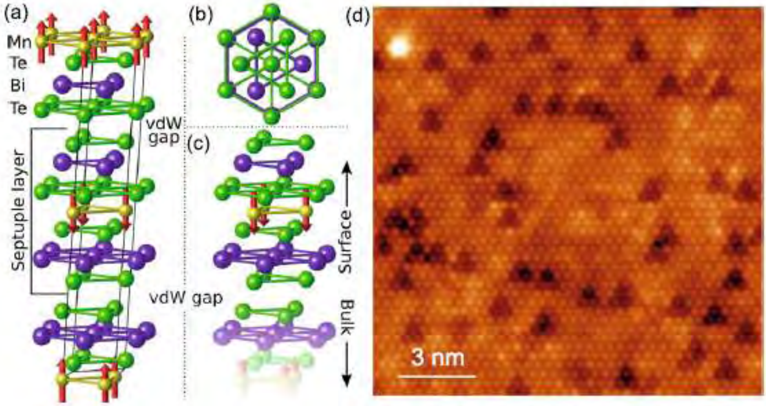

Figure 1: **$MnBi_2Te_4$ bulk and surface structure**. **a)** Side view of the bulk crystalline structure of $MnBi_2Te_4$ with red arrows showing the interlayer AntiFerroMagnetic order. The crystal cleavage in this layered compound takes place at the van der Waals gap, thus exposing a Te layer of a Septuple Layer at the surface. **b**) Top and **c)** side views of the surface crystal structure. **d)** Atomically-resolved STM image of the surface of the cleaved sample (1 V and 0.3 nA) showing the hexagonal aarray of Te atoms and some defects (dark triangular depressions and a bright circular protrusion).

Magnetic 2D materials: studying and manipulating ordered spins in flatland.

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Layered materials have been at the heart of the field of magnetism since the pioneering observations of antiferromagnetic phase transitions more than a century ago. The manifestation of spontaneous magnetization in two dimensions has thereafter captured the attention of condensed matter physicists. From a theoretical point of view, the Mermin and Wagner theorem demonstrated that long-range ordering in low dimensions is forbidden in an isotropic spin lattice. In order to confirm this theorem, many experiments were performed in the layered magnetic materials as model two-dimensional (2D) spin lattices. However, despite the layered nature, interlayer coupling in bulk systems is not negligible and an approach for the study of true 2D magnetism had been lacking until the avenue of 2D materials. In this talk, I will start by reviewing the long history of magnetism in 2D systems, culminated by the realization of long-range magnetic order in a 2D material with the discovery of the first free-standing ferromagnetic 2D material made out of a single layer of chromium triiodide (CrI_3) [1]. The pioneering experiments on CrI_3 showcase the dramatic layer dependence and non-trivial exchange interactions of the magnetic ground states in atomically-thin van der Waals crystals down to the monolayer. In particular, an intriguing metamagnetic behaviour emerges in CrI_3 as the ferromagnetic bulk is thinned down, which might have its ultimate origin in a unique mesoscopic layer-dependent structural phase transition [2, 3]. Finally, I will highlight the potential of this new class of few-layer magnets for developing efficient magneto-optic [4], magnetoelectric [5], magnetoelastic [6] and spintronic devices [7], and for the study of competing strongly correlated states in two dimensions.

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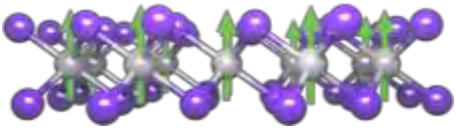

Figure 1: Cartoon representation of single layer CrI_3, portraying the long-range out-of-plane order of the spins in the lattice below the Curie temperature.

π-Magnetism inf Engineered Graphene Nanostructures

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Graphene can spontaneously develop intrinsic paramagnetism. Some examples are the emergence of spin-polarized bands in zig-zag edges in graphene, or the observation of magnetic moments in open shell graphene nanostructures. Radical states at the conjugated lattice, as singly occupied states, respond to the presence of finite electron correlations by localizing in certain sites and gaining a net spin polarization. The interesting aspects of this unconventional form of (para)magnetism is that it is part of the conjugated lattice of graphene. Therefore, it extends for nanometers length scales, and interact with others with exchange coupling strengths of tens of millielectronvolts. The challenge of fabricating atomically precise graphene structures with custom shapes for localizing spins and tuning their interactons became possible with the development of on-surface synthesis.

In this presentation, I will show results on spin-hosting nanographenes, including their syntesis routes, their magnetic fingerprints and the origin of such unconventional form of magnetism. We use scanning tunneling microscopy and spectroscopy to detect and spatially localized the spin density by mapping the amplitude of a Kondo resonance [2,3,4,6] or spin excitations [2,5].

One of the most paradigmatic systems for graphene magnetism is Triangulene. These triangular pieces of graphene with zigzag edges exhibit high spin due to frustration of their conjugated lattice [4]. Doping the triangulene with heteroatoms can modify the spin state [6]. However, as we shall show, the charge balance of graphene nanostructures with metallic substrates can also modify their spin state due to new orbital filling configurations. Traingulene can also be connected by covalent bonds and their intrinsic spin state survives. In particular, we found that a Triangulene hexamer ring (see the figure), fabricated by combining solution and on-surface syntesis, exhibits fingerprints collective spin states [4]..

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Figures

Atomic force microscopy images carry chemical information: Halogen bonds, Tautomerization, and molecular identification with deep learning

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High resolution non-contact atomic force microscopy (HR-AFM) with CO-functionalized metal tips reveals the internal structure of adsorbed organic molecules with unprecedented resolution, resolving intermolecular features, determining bond orders, and characterizing intermediates and final products generated in on-surface reactions [1].

Here, we show how the chemical information imprinted in HR-AFM images paves the way for understanding how the molecule-substrate interactions can be exploited to tune (i) the strength and the directionality of intermolecular halogen bonds [2], (ii) the nature and energy barriers for tautomerization in meso-Dibenzoporphycene (mDBPc) molecules [3], and (iii) the hydrogen bond driven molecular self-assembly in the paradigmatic case of trimesic acid (TMA) molecules [4]. Furthermore, we demonstrate that HR-AFM images contain enough information not only to reveal the molecular structure but also to identify each atomic species. This identification can be automated with machine learning techniques, using neural networks trained mainly with a large dataset of theoretical AFM images [5,6].

Regarding halogen bonds [2], we present an approach for controlling the 2D self-assembly process of halogenated compounds by adsorption on reactive metal surfaces. Molecule-substrate interactions modify the strength of the σ-hole, a positive region at the caps of the halogens, reversing the order of halogen bond strengths known from gas phase. Adsorption of mDBPc, dominated by the metal-coordination bond of the lone-pair electrons of the imine N atoms with the substrate, results, on NaCl films, in a new type of tautomerization process, where the transfer of H atoms within the porphycene cavity is accompanied by a significant displacement of the whole molecule [3]. Accurate comparison between modeled images and experiments on TMA on Cu(111) [4] allows us to identify key structural elements in the assembly in terms of the electron-withdrawing character of the carboxylic groups, their interactions with the surface, and the electron density in the region of the hydrogen bonds.

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Charge Matching of occluded Organic Structure Directing Cations in Zeolites

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Organic Structure Directing Agents (OSDAs) play a central role in synthesis of zeolites. Typically, OSDAs consist in tetraalkylammonium cations that are trapped inside of the voids of zeolites. The positive charge of the occluded cations is compensated i) by the isomorphic substitution of Si atoms by trivalent atoms resulting in negatively charged zeolite framework; ii) by the presence of framework defects consisting in the Si-O- species and Si-OH (silanols) and iii) by the incorporation of fluoride anions in small zeolite cages. The charge compensation method depends on the synthesis gel composition and crystallization conditions.

The exact location of the occluded OSDA has been matter of interest because it is accepted that there is a pairing between the negative zeolite and OSDA positive charges in order to maximize coulombic interactions. Thus, the distance between the highest positive charge density of the OSDA (typically on the N atom) and the negative charge associated to presence of T(III) atoms, Fluoride anions or defects must be as short as possible. This is call the charge matching effect.

Additionally, the occluded OSDA must fit inside of the voids of the zeolite and it is accepted that Van der Waals interactions drive the crystallization of zeolite towards the particular structure that host the OSDA. Thus, the final structure of the zeolite will depend on both effects, charge compensation and host-guest interactions.

In this presentation, we will introduce a new parameter in the understanding of zeolite crystallization and is the possibility of stablishing different configurations of OSDA-zeolite for charge compensation. This may drive to different location of the active acid sites in the final zeolite, which has been found to be relevant in improving catalytic performance of microporous materials.
For illustrating this idea, we will present a new zeolite, named ITQ-66, which can be synthesized as Borosilicate and Gallosilicate but not as Aluminosilicate. Depending of the final composition, B or Ga are located at different T-sites of the zeolite structure and therefore, charge compensation occurs in a different manner.

Also, we have found that compensating fluoride anions can ‘jump’ from one particular crystallographic location to another during the course of crystallization or just by gentle heating of pure silica RTH samples. Again, charge compensation of the occluded OSDA cations could take place by negative charges placed at different crystallographic positions.

These findings make us to conclude that charge matching mechanism is not a biunivocal relation between positive and negative charge locations. Here, we have found that inorganic compensating defects (i.e. T(III) or interstitial F anions) may be placed at different locations in the zeolite structure in presence of the same OSDA.

Hollow nanoparticles: applications in nuclear fusion power plants

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In the last years, hollow nanoparticles have been studied due to their astonishing properties. In particular, their high resistance to elevated temperatures and pressures and their distinctive optical properties. Fabrication is an issue for many materials due to the natural trend of the nanoparticles to the most stable configuration, the solid sphere. In this talk, a brief description about fabrication methods by means of laser pulses will be given to focus next on the application of hollow tungsten nanoparticles in future nuclear fusion power plants. The first wall of these plants is still an open problem in many concepts due to the poor behaviour of the existing plasma facing materials under the expected detrimental irradiation conditions. A special concern is related to the retention of light species, in particular hydrogen and hellium. Our studies on tungsten hollow nanoparticles under different irradiation scenarios by means of classical molecular dynamics determined that these particles can resist temperatures up to 3000 K and huge internal pressures (>5 GPa at 3000 K) before rupture. In addition, a self-healing mechanism leads to the formation of an opening, through which gas atoms are able to escape. The opening disappears as the pressure drops, restoring the original particle. By means of object kinetic Monte Carlo simulations we found an additional self-healing mechanism for defect annihilation. We will discuss our multiscale methodology and the results obtained for different fusion scenarios. We will show the promising behaviour of hollow tungsten nanoparticles in some scenarios, which opens a new path to solve a long-standing problem in the field of fusion technology.

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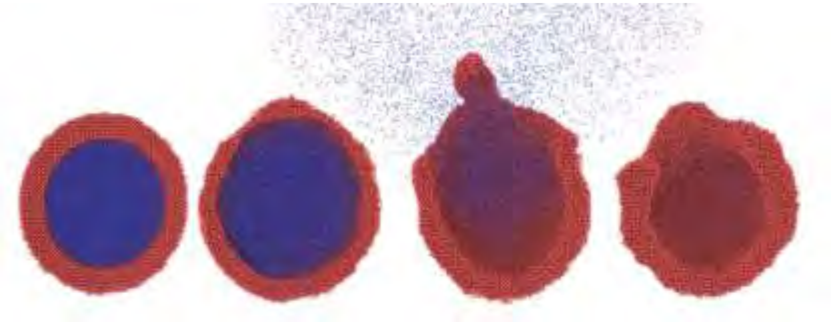
Figures



Molecular dynamics simulations of a hollow tungsten nanosphere explosion highly pressurized at 3000 K. Red = W atoms, Blue = Helium atoms.

Amorphous Materials for Applications in Nanoelectronics and Neuromorphic Computing

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Abstract

The fabrication and characterization of disordered materials has recently witnessed an outstanding progress leading to materials with unprecedented properties. In particular, the possibility to synthesize wafer-scale two-dimensional amorphous carbon monolayers, structurally dominated by sp^2 hybridization, has been demonstrated. This achievement has initiated a new platform of low-dimensional materials allowing to explore alternative forms of membranes with enhanced chemical reactivity which could be employed for instance in advanced coating materials [1,2].

The excellent physical properties of the mentioned materials derive from the nature and degree of their disorder which, controlled at the fabrication level, represents the key ingredient to tune their physical/chemical properties for specific target applications. In this respect, new fabrication strategies to modify the degree of disorder and a systematic theoretical characterization of the impact of the material structural quality on the ultimate performance is urgent. Even more importantly, the search for new disordered materials for novel applications appears as an extremely promising way. In this talk we present a systematic analysis of the structural, vibrational and electronic properties of amorphous carbon monolayers as a function of the structural quality of the material. We show how disorder results in a tunable electrical conductivity and thermal properties [3]. Finally, we present the results of the newly demonstrated synthesis of a thin film of amorphous Boron Nitride showing extremely low dielectric characteristics: high breakdown voltage and likely superior metal barrier properties [4]. The fabricated material aims at replacing current interconnect insulators in the next-generation of electronic circuits. We discuss the experimental setup and present the results of our calculations which have contributed to the understanding of the structural morphology of the amorphous material. We conclude discussing the resulting thermal and electronic properties [5] and the applications in neuromorphic computing.

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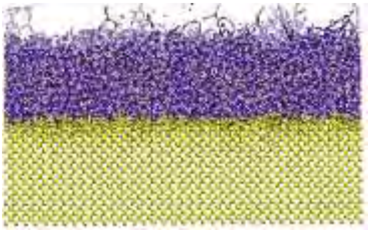

Figure 1: In silico growth of a thin film of amorphous Boron-nitride (60% sp^2)

Exploring new 2D halides materials for quantum devices

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The recent evolution at building quantum devices, especially quantum computers, is requiring important developments on hardware optimization with the potential to solve problems that cannot be solved by classical computers. The scaling up of the quantum processors requires improvement of the qubit's performance that stimulates investigation of alternative architectures and new pipeline of materials that also allows controlling and reducing the noise, loss and decoherence process of present devices. Among the new arquitectures and materials that are being explored as new platforms for future developments, creating heterostructures based on two-dimensional materials grows day by day, with special attention on those including magnetic semiconductors suitable for creating exchange coupling in the heterostructures with superconductors.

In this context, by combining different highly sensitive surface science technique, we are exploring the magnetic, electronic and structural properties for binary transition metal dihalides MX_2 (M=Metal cation, X=halogen anion) which theoretically exhibit promising magnetic and electronic properties. We demonstrate that these MX_2 (M=Ni, Fe, Co; X=Br, Cl) materials, that can be epitaxial grown on different substrates [1], present ferromagnetic ordering (collinear or non-collinear depending on the compound) in the limit of a single or a few atomic layers thick films, although in bulk form they are antiferromagnets. Moreover, we also probe the survival of superconductivity when these materials are in contact with a superconductor material, such as $NbSe_2$ or Al. The advantage of these materials compared to other 2D materials, such as graphene or TMDs, is that their synthesis is compatible with standard microelectronic manufacturing (lithography, resin prepattern, etc) and, therefore fabrication of devices does not require any exfoliation or stamping of the 2D flakes.

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Figures

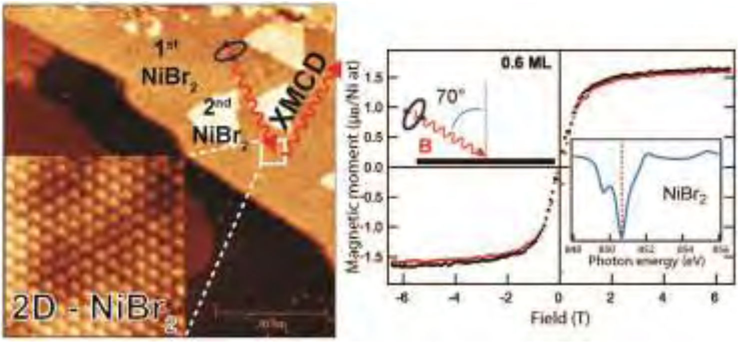

Figure 1: STM image and XMCD Magnetization loop measured for $NiBr_2$ epitaxially grown on Au(111) both measured at temperatures around 4K (XMCD magnetization loops measured for L3 Ni edge varying the magnetic field).

Personalized in vitro extracellular matrix models using nanoparticles or cell-derived matrices.

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The question of how exactly cells sense their environment (including the extracellular matrix and neighbouring cells) and respond to it has fascinated scientists for decades. Indeed, we know that environmental inputs can drive cells into distinct paths such as division, differentiation, and even malignancy, representing a paramount regulator of cell function in a myriad of physiological settings. Therefore, by deepening our fundamental understanding of cell-matrix interactions, researchers also contribute to the development of therapies or devices to tackle injury and disease across our bodies.

Since cells exist in the micro-world, their interactions with the surrounding matrix take place primarily at the nanoscale. Protein receptors at the cell membrane bind to ligands present in extracellular proteins; these adhesions have intracellular repercussions and regulate parameters such as cell shape, cytoskeletal organization, or gene expression. Therefore, it is relevant to study the ECM architecture in patients' tissues and to identify biomarkers useful for their diagnosis, prognosis, and guidance of therapeutic intervention. The role of ECM fibrillar organization is increasingly investigated and analysed through the various imaging techniques and associated quantification tools. In this work we will focus on one part to produce nanopatterns of cell-binding ligands and employ them as in vitro platforms for mesenchymal stem cells, in culture media inducers of differentiation towards cartilage, tendon or bone. We analyse cell movement dynamics, the formation of early tissue structures and their mechanical properties and stability, intercellular communication, and cell differentiation to each of the lineages. In a complementary way, we examined the properties of ECM fibres and fibril bundles in patients' and model tissues obtained from cell derived matrices. We focused on Collagen VI related muscular dystrophies (COL6 RMD) because these pathologies present a clear link between altered ECM architecture and patients' outcome. The results obtained confirm that unveil fundamental cell-matrix interactions that drive the development of musculoskeletal tissues can be exploited at clinical level

Porous Silicon Arrays as a Playground for Microbes

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The attachment of microorganisms, bacteria and fungi, to abiotic surfaces is of great interest to both the scientific and medical communities and numerous new methods and materials for quantitatively examining bacterial attachment and colony formation on surfaces have recently emerged. Intriguingly, most works have explored micro-/nano-structured substrates as potential antimicrobial surfaces, with an emphasis on antibiofilm properties; whereas, fewer have studied such patterned surfaces as artificial microbial arenas for observing and elucidating the behavior of bacterial communities.

Using engineered porous silicon substrates with carefully designed nano/micro topographies, exhibiting photonic properties, we introduce an optical platform that enables real-time and label-free monitoring of bacterial surface adhesion and colonization. Thus, the porous substrates serve as both a preferable solid-liquid interface for microorganisms networking and a simultaneous transducing element that monitors their response. Such platforms do not require sophisticated microscopy tools or any labels as most of the currently used methods, and it can be conveniently modified with different topographies and surface chemistries, presenting endless study opportunities in a single tool. We demonstrate the application of these platforms to study how different bacterial species, ranging from standard laboratory strains to genetically engineered mutants and clinical isolates, preferentially colonize surfaces with varying topography, wettability and charge and monitor over the formation of a biofilm. Moreover, we employ these manipulated porous surfaces for solving some critical bottlenecks in clinical microbiology [1]. For example, we have developed a chip-based culture-free method for rapid screening of resistant/susceptible bacteria directly from a clinical sample within only 90 minutes, where current clinical state-of-the-art methods require at least 24 hours [2-3].

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Intrinsic Properties of Multiphase Nanostructured Ionic Conductors

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Abstract

Multiphase polymeric nanostructured conductors are of continued interest for their potential application in electrochemical systems. Multiphase materials can enable advance properties that cannot be achieved without structure. The effect of the nanostructure on ionic transport, charge transfer, and interfacial process, however, can be complex due to the inability of traditional 'bulk' experiments to directly correlate between the ionic phenomena and the structure properties. I will demonstrate that by using advance polymerization, self-assembly and nanofabrication methods we can design structured systems with deterministically defined ionic pathways, interfaces, and chemophysical properties that enable us to isolate, visualize and quantify ionic phenomena at the nanoscale level.

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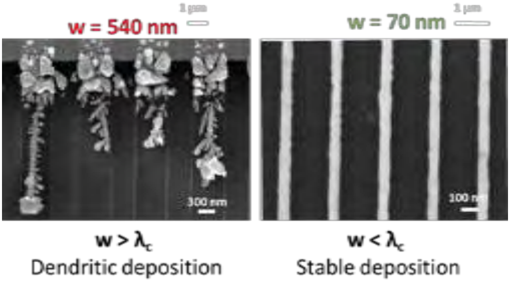

Figure 1: Stabilizing dendritic growth by nanostructured ionic conductors

Polypeptide-based Nanoconjugates as Versatile Therapeutics

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Polypeptides are already playing a major role on a number of different relevant areas such as nanomedicine [1]. The physico-chemical parameters of a polypeptide-conjugate, and hence its biological performance, are defined by an intricate interplay of multiple structural factors. This highlights the need for detailed structure-activity relationship studies to develop the hierarchical strategies of polypeptide conjugate design. However, structural complexity also represents a unique opportunity, since small changes at the structural level might endow nanomedicines with outstanding and unexpected biological performance [1].

In our group, we have overcome the main classical limitations for the synthesis of defined polypeptides using precise controlled reactions followed by an adequate characterization yielding to well-defined polypeptidic architectures by NCA polymerization techniques [2]. In addition, post-polymerization techniques allow us the introduction of a variety of functionalities yielding a set of orthogonal reactive attachment sides [1,3]. Using these techniques and following a bottom-up strategy we have been able to obtain star-based polypeptide architectures with the capacity to self-assemble yielding supramolecular nanostructures with interesting properties [4]. This strategy together with an adequate polymer-drug linker design [5] enabled in vitro and in vivo evaluation, revealing a lack of toxicity, an enhanced in vitro cell internalization rate and significantly greater terminal and accumulation half-life in vivo together with a significant lymph node accumulation [4]. These results allow us to envisage these systems as promising nanocarriers for therapeutic or diagnostic applications, especially in anti-cancer treatments including lymph node metastasis and cancer immunotherapy. Proof of Concept for metastatic breast cancer [5] and for immunotherapy design in melanoma will be also shown as well as the use of this self-assembled architectures in applications such as neurodegenerative disorders [6], spinal cord injury [7] or acute kidney injury [8].

Acknowledgements

This work has been supported by European Research Council (grant ERC-CoG-2014-648831 “MyNano”, Grant ERC-PoC-2018-825798 Polymmune), the Spanish Ministry of Science and Innovation (SAF2016-80427-R, PID2019-108806RB-I00), Fundació Marató TV3, Fundación Step by Step and Agencia Valenciana de Innovación (AVI) INNVAL10/19/047. Part of the equipment employed in this work has been funded by Generalitat Valenciana and co-financed with FEDER funds (PO FEDER of CV 2014–2020).

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State-of-the-art in imine-based covalent organic frameworks processability

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Covalent Organic Frameworks (COFs) are porous and ordered organic materials formed by simple condensation reactions of organic molecules. Recently, the Schiff-base chemistry or dynamic imine-chemistry has been explored for the synthesis of new COFs. The main reason for this tendency is the higher chemical stability, porosity, and crystallinity that they show in comparison to those previously reported, e.g. boronate ester-based COFs [1].
This talk will summarize the most recent progress in preparing imine-based COFs that enable their processability [2]. I have selected some recent examples on 3D-printing of imine-based COFs [3] and imine-based COF gels' formation and their transformation into aerogels and films to form functional centimeter-long membranes [4,5]. I will provide some perspectives on potential applications of these materials.

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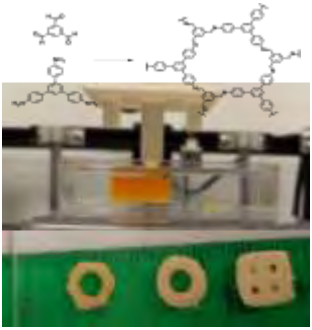

Figure 1: 3D Printing process of a prototype imine-based COFs and several shapes obtained after activation process.

INVITED SPEAKERS

Living on the edge: 1D van der Waals materials by design for nanophotonic applications

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The fabrication of 2D materials such as transition metal dichalcogenides (TMDs) in geometries beyond the standard platelet-like configuration exhibits significant challenges which severely limit the range of available morphologies. Furthermore, industrial applications based on TMD nanostructures with non-standard morphologies require full control on the size-, morphology-, and position on the wafer scale. Such a precise control remains an open problem of which solution would lead to the opening of novel directions in terms of optoelectronic and nanophotonic applications. Here we present recent studies on a novel strategy to fabricate position-controlled nanopillars (NPs) based on TMDs materials at the wafer scale [1]. Realizing the precise localization of the TMDs NPs enables a highly localized nonlinear signal required for many nanophotonic applications. Furthermore, an in-depth study of the local electronic properties of such TMD nanomaterials with non-standard geometries requires the combination cutting-edge transmission electron microscopy techniques with machine learning. I will describe the EELSfitter STEM-EELS data analysis framework [2] which makes possible the spatially-resolved determination of crucial properties of TMD nanomaterial such as the bandgap and the complex dielectric function.

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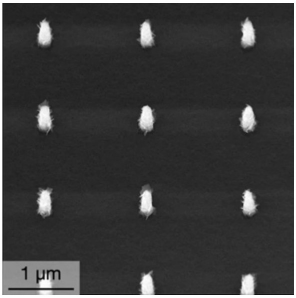

Figure 1: Scanning electron microscopy of 1D array of TMD-based nanopillars.

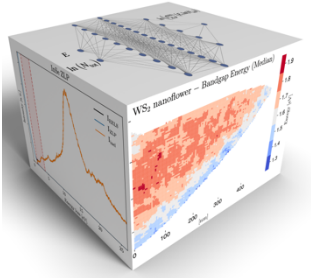

Figure 2: Machine learning for EELS data interpretation

Design of functional nanopatterned porous ferroic metal oxides

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Perovskites and ferrites materials are important ferroic materials which may find application in several fields including ultrafast data reading, enhanced storage capacity, laser-assisted electronic data recording in ferroelectric memories, catalytic materials, and sensor devices. Nanopatterning porosity may be a tool to modify the properties of metal oxide thin films. In CICECO - Aveiro Institute of Materials, we have been focused on the understanding of the porosity effect on the piezoelectric properties of thin films. Nanoporous thin films of lead titanate [1,2] and bismuth ferrite [3], as examples of oxides with perovskite and ferrite structures, were prepared by block-copolymer self-assembly (Figure 1). Films with different thicknesses and pore organizations were also prepared. The films were characterized in relation to the structure and morphology by X-rays diffraction, scanning electron microscopy and atomic force microscopy. The electric properties were measured at nanoscale by piezoelectric-response force microscopy and are compared with dense counterparts with similar thickness. Nanopatterned PbTiO3 films present higher switchable polarization and $(d33)_{eff}$ piezoelectric coefficient than dense thin films (137.6 ± 6.7 pm/V and 49.6 ± 0.7 pm/V versus 85.1±2.0 pm/V and 35.7±0.8 pm/V, respectively), demonstrating the positive effect of porosity on the enhancement of the ferroelectric properties. Nanopatterned $BiFeO_3$ layers with 66 nm of thickness and average pore diameter of 100 nm at 600 °C were prepared. The large vertical porosity markedly enhances the local electric and macroscopic magnetic properties when compared with the dense counterparts. The vertical porosity orients the piezoelectric domains and reduces the energy necessary to reorient the dipoles. The induced instability in the dipole-dipole interactions results in the increase of the effective piezoelectric coefficient.

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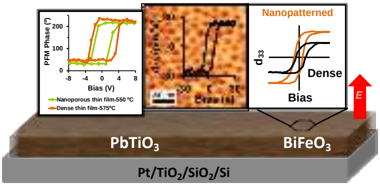

Figure 1. Nanoporous $PbTiO_3$ and $BiFeO_3$ thin films.

Acknowledgement

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Design and realization of heavy-fermion quantum matter in van der Waals materials

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Van der Waals materials have allowed realizing a variety of emergent quantum states, including topological phases and unconventional superconductors. However, heavy-fermion correlated states, usually found in complex rare-earth compounds dominated by Kondo physics, have remained elusive in the two-dimensional world. The realization of heavy-fermion physics in two-dimensional materials would provide a whole new playground to explore exotic forms of quantum criticality, quantum magnetism, hidden order, and unconventional superconductivity. Here we show that van der Waals materials based on graphene and transition metal dichalcogenides allow realizing heavy-fermion states without rare-earth elements. First, we will theoretically show [1] how a heterostructure solely based on three layers of graphene allows realizing a tunable heavy-fermion state, whose full Doniach phase diagram can be explored by means of an interlayer bias. Second, we will show [2] the design and experimental realization of a heavy-fermion state in a 1H-TaS2/1T-TaS2 twisted dichalcogenide bilayer. Our results bring the physics of heavy-fermion rare-earth compounds to the two-dimensional world, opening a pathway towards designing and controlling a whole new family of correlated physics in moire van der Waals heterostructures.

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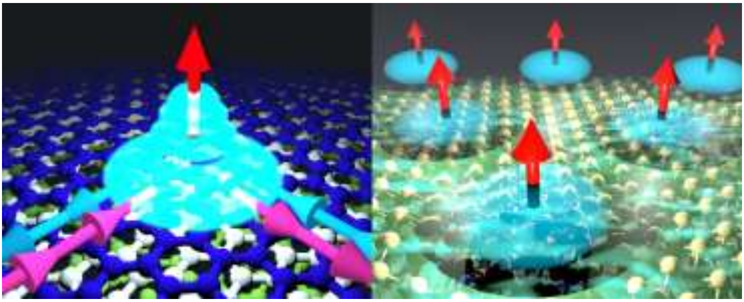

Designing of nanoporous anodic alumina photonic structures and applications

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Nanoporous anodic alumina (NAA) has become an interesting material because of their outstanding set of properties, cost-competitive fabrication processes and fully scalable process compatible with conventional micro- and nanofabrication technology. NAA is obtained by the electrochemical etching of aluminum. [1-3]. Recently, different anodization and post-anodization treatments have been developed to create new structures and pore geometries such as modulated, funnel-like, serrated-like, tip-like, etc. The application of periodic variations of current or voltage during the anodization is transferred to the material as the periodic variation of the pore diameter and consequently, it is possible design, 1D, 2D and 3D structures. It is very interesting the design photonic structures (PS) with tunable stop bands within the UV-VIS-NIR range by applying cycling anodization processes [4-6]. Motivated for these excellent properties in this work, we present the recent advances of different photonic structures with different anodization approaches. Figure 1 shows an example of a sinusoidal current profile and involved parameters during the fabrication. Figure 1b shows the characteristic reflection spectrum of the Photonic structures. FESEM images shows the top view of the PS-NAA it is observed the nanopores distributed randomly on the surface of the sample (figure 1c) and the cross-section showing the pore modulation along the depth (inset).

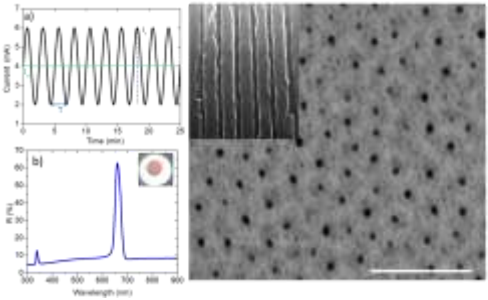

Figure 1. Sinusoidal anodization profile of Photonic Structures and involved anodization parameters. (b) Reflection spectrum of Photonic structures with sinusoidal anodization profile, (c) ESEM top view of the NAA-PS and ESEM cross-section of NAA-PS. Scale bar 1 µm.

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Laser bioprinting using BA-LIFT: from single cell to tissue engineering

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Laser bioprinting techniques are appearing as an ideal tool for cell printing due to their outstanding cell viability (near 100 %) and high spatial resolution (in the micrometer range). In this paper we discuss different applications of a particular adaptation, made at Laser Center UPM, of the Blister-Actuated Laser Induced Forward Transfer (BA-LIFT) technique [1] for cell printing. In our case we use a thick polyimide layer for blister generation to protect the cells from the incomimg laser beam. Due to the transparency of this material in the VIS range we can implement both fluorescence and conventional vision systems coaxially with the laser path in order to identify the cells to be transferred, opening up the possibility of cell sorting [2]. We discuss some current applications of the technique developed at our lab, from single cell isolation to applications in tissue engineering. In addition we present lateral images of the transfer process obtained with a high speed vision camera in order to discus the dynamics of the jet generation and cell deposition mechanisms in the acceptor substrate.

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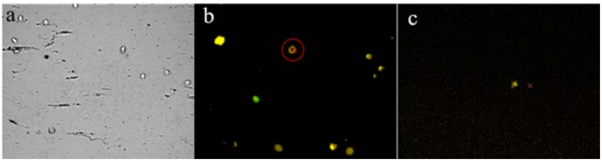

Figure 1: (a) Donor layer bright field image showing mixed cells (b) Donor layer fluorescence image showing mixed cells, Jurkat cells (α-CD45/PE) are shown in yellow and C1R-N1-85 are shown in green. (c) Acceptor layer fluorescence image showing a Jurkat cell (α-CD45/PE) after isolation process

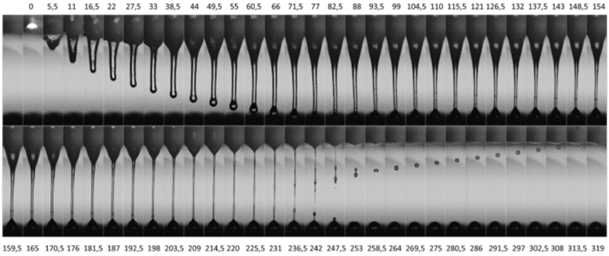

Figure 2: Complete sequence of jet formation an cells transfer. Frames are shown every 5.5 µs.

A new Formula based EBL Nanopatterning Approach for large Metalens Fabrication

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Metalenses with a high numerical aperture and high efficiency have gained widespread attention in both academia and industry due to their ultra-flatness, compact size, and high-resolution imaging quality. These features qualify metalenses for potential future integration in common everyday products such as cellphones, cameras or bio-diagnostic, augmented and virtual reality components. The basic unit blocks of metalenses are typically subwavelength spaced nanostructures, such as nanofins, nanorods, and nanocylinders. These nanostructures are designed across the substrate with varying rotation angles or sizes, depending upon the design of the optical properties and specific planar position of these structures. Since high precision placement of shapes and good minimum line edge roughness (LER) definition are essential for the fabrication of these nanostructures, electron beam lithography (EBL) has been widely used for patterning. Due to the large number, complexity, and only minimally varying rotation angles of the features, exposing such patterns poses significant challenges on EBL in terms of pattern fidelity and throughput.

Corresponding conventional GDSII designs can easily exceed several 100MB if not TB of design data file size, something that is extremely demanding for the classical data processing paths of the EBL tool. Even if the amount of data can be handled at all, typically a lot of overhead is generated as well such that exposure times can get extremely unattractive.

In order to circumvent this situation and to totally avoid the necessity to create a flat GDSII design file, two alternative approaches of formula based, lean data generation and processing have been implemented in the dedicated Raith EBL systems EBPG and VOYAGER. This has been accomplished by creating the exposure data algorithmically based on scripts [1,2] or C programming respectively. Applying this method, large area metalenses with cm-dimension were fabricated while increasing throughput by factors of~10.

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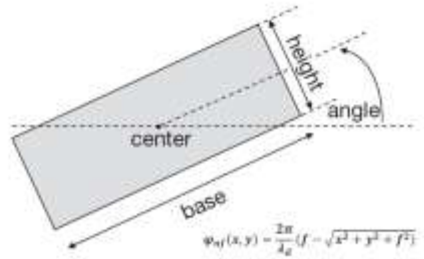

Figure 1: Definition of a cube shape (nanofin) used for algorithmic patterning of a metalens. The angle rotation can be changed in the nano degree regime.

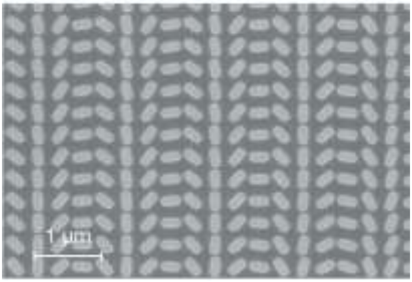

Figure 2: SEM images of the metalens pattern in 100 nm ZEP520 A resist on a silicon substrate.

Surface acoustic waves in graphene & 2D materials for manipulating light-matter interactions

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Surface acoustic waves (SAWs) are especially well suited for modulating graphene and other 2D materials as their strain and piezoelectric fields are strongly concentrated at the surface of the piezoelectric substrate that supports the 2D crystal. Moreover, many 2D materials are themselves piezoelectric, enhancing the capabilities of strain modulation. The interdigital transducer (IDT) technology permits to excite the SAWs electrically to generate strain locally at very high frequencies, as shown in figure 1. In this talk, we will first demonstrate that this strain allows to modulate dynamically the optical and vibrational properties of graphene, as proven by the change on its Raman signature [1]. Second, we will show that SAWs also provide an outstanding platform for confining light at the nanoscale, exploiting the strengthening of its associated electric field, which results in enhanced light-matter interactions or quasiparticles. Thus, the strain field of the SAW can create a dynamic optical grating allowing to launch propagating polaritons in unpatterned graphene and other 2D materials. In particular, we will present the generation of SAW-driven surface plasmon-phonon polaritons in graphene and graphene/h-BN systems [2, 3], the latter also supporting hyperbolic modes. Finally, we will show how this concept can be generalized to stacks of 2D semiconductor materials (for example MoS_2 and black phosphorus) on thin metal layers, where the SAW generates surface plasmon-exciton polaritons (or plexcitons) [4]. These SAW-mediated architectures pave the way for implementing nanophotonic devices and biosensors, where polaritons can serve as ultrafast and low power signal carriers and ultrasensitive probes, respectively.

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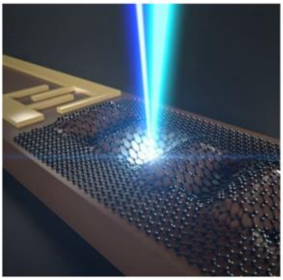

Figure 1: A SAW generated with an IDT deforms the graphene (or other 2D crystal) locally and dynamically to manipulate the properties of the material and/or the light-matter interaction.

Harnessing the structural modulations in van der Waals heterostructures by 4D-STEM nanodiffraction

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The physical properties of two-dimensional materials are highly sensitive to structural distortions such as ripplings or corrugations that produce large strain fields. These effects can be enhanced in van der Waals heterostructures, such as the naturally occurring franckeite, in which the mismatch between its constituent pseudohexagonal and pseudotetragonal two-dimensional layers gives rise to a spontaneous rippling that is responsible for a strong anisotropy of the electrical, vibrational, and optical properties of the material [1]. Moreover, small variations in the multilayered structure and composition of this material can give rise to a strong topological insulator phase [2]. Understanding the complex structure of such materials, specially in its 2D state, is thus of high interest due to their potential applications in new electronic and optoelectronic devices. Here we show how four-dimensional scanning transmission electron microscopy (4D-STEM) nanodiffraction allow us to map the local structural modulations occurring in the van der Waals heterostructure Franckeite and characterize the strong strain fields arising from a 3D structural rippling. We measure a full 2D image of the transmitted electron beam, or a convergent beam electron diffraction pattern (CBED) as the electron beam is raster scanned over a 2D grid of probe positions in real space, as schematized in Fig. 1, and gather new information about the spontaneous rippling and strain modulations in this material. 4D-STEM brings thus a new pathway to study the structural and physical properties of 2D materials and heterostructures.

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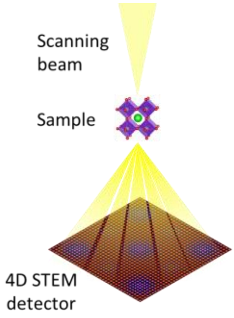

Figure 1: Schematic of a four-dimensional scanning transmission electron microscopy dataset showing the convergent beam electron diffraction patterns acquired as the probe is raster scanned across a 35×35 grid to image a $SrTiO_3$ unit cell in the [001] orientation.

Acknowledgements

We thank Andrés Castellanos-Gómez for providing samples. G.S.-S. acknowledges financial support from Spanish MCI Grant Nos. RTI2018-099054-J-I00 (MCI/AEI/FEDER, UE) and IJC2018-038164-I. F.F.-C. and M.V acknowledge financial support from Spanish MICINN RTI2018-097895-B-43 (MCI/AEI/FEDER/UE).

Moiré physics in 1D and 2D

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Moiré patterns emerge when two periodic structures are overlaid and fully charachterized by the twist angle between them. The resulting material is a new entity and exhibit emergent properties, drastically different from those of their components. In this talk we address the questions: what are the further degrees of freedom that emerge when moving from 2D to 1D? Are these experimentally accessible and usable in nano-devices? How do the combined effect of twist angle and strain modify the hybrid material properties in 2D?

To answer these questions, we investigate interference effects in finite sections of 1D moiré crystals using the Landauer-Büttiker formalism within first-principles and tight-binding approximation [1]. We address interlayer transport in double-wall carbon nanotubes and demonstrate that wave function interference is visible at the mesoscale: in the strong coupling regime, as a periodic modulation of quantum conductance and emergent localized states; in the localized-insulating regime, as a suppression of interlayer transport, and oscillations of the density of states. The interlayer transmission between strongly coupled metallic nanotubes is limited to either $1G_0$ or $2G_0$. Our results could be exploited to design quantum electronic devices, e.g. non-electric switches based on chiral nanotubes. Most importantly, we clarify the origin of the so-far unexplained $1G_0$ quantum conductance measured in multi-wall carbon nanotubes [2, 3]. Further, we show that the relative orientation angle between graphene and TMDs can be exploited to tune proximity induced SOC in graphene and create ideal conditions for next-generation memory storage based on spintronics [4].

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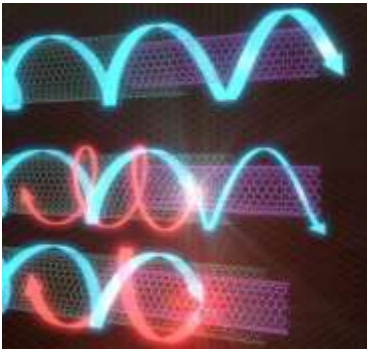

Figure 1: Quantum Conductance in double wall CNTs can proceed undisturbed and plateau to the conductance quantum (G_0), partially transmitted, or completely blocked, depending on the spatial overlap of the two carbon nanotubes and their nature (chiral vector). Image: Damaso Torres, ICN2 Barcelona.

ORAL CONTRIBUTIONS

Magnetism in Transition Metal Ilmenenes

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Abstract

Ilmenene is a new two-dimensional material that has recently been exfoliated from the naturally occurring titanate ore ilmenite (FeTiO3) [1], a material found in abundance on the earth´s surface. With the synthesis of this material, it is a matter of time before other similar systems are obtained from their bulk counterparts. In this work, using density functional theory, we performed calculations of the structural, electronic and magnetic properties of the ilmenenes $TMTiO_3$ (with TM running from V to Zn), being more stable when they are TM ended. The magnetic ground state is antiferromagnetic, except for the Cu and Zn cases which shown ferromagnetic and spin compensated solutions, respectively. The energy differences with respect to the ferromagnetic system are about 0.01 eV/TM-atom, although for the Cr and Cu ilmenenes the differences become considerably larger. The TM local magnetic moments as a function of the atomic number follow the Slater-Pauling type curve. We established a simple electronic model filling the TM levels. However, for the Cr and Cu cases, we find a Janh-Teller like distortion breaking the degeneracy of the dxz and dyz orbitals. Because magnetism in two-dimensional materials is being currently held promising for spintronics, the synthesis of these materials could be interesting for experimentalists.

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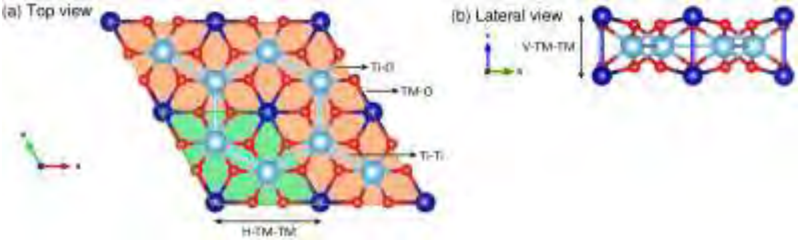

Figure 1: Top (panel (a)) and lateral (panel (b)) view of transition metal ended ilmenene-like systems.

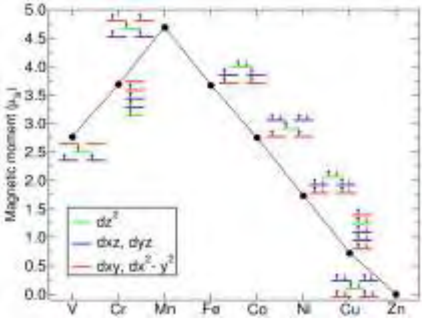

Figure 2: Calculated local magnetic moment at the transition metal atoms. For each compound, the electronic filling model is also shown. Red levels denote the in-plane $dx^2–y^2$ and dxy orbitals; green, the out-of-plane dz^2 orbital: and blue, the orbitals dxz and dyz.

Engineering of Charge Current Flow in Nanoporous Graphenes

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During the last decade, on-surface fabricated graphene nanoribbons (GNRs) have gathered enormous attention due to their semiconducting π-conjugated nature and atomically precise structure.[1] GNRs are regularly characterized by means of scanning probe microscopy (SPM), which has also allowed to study exotic electronic quantum phases realized in these nanostructured materials.[2] A significant breakthrough in the same field was the recent fabrication at ICN2 of nanoporous graphene (NPG) as a 2D array of laterally bonded GNRs.[3] This covalent integration of GNRs could enable complex electronic functionality at the nanoscale, with the ability to tune the electronic coupling between GNRs within NPGs. In this talk, I will present our recent works, based on quantum chemical calculations and large-scale transport simulations, and in which we demonstrate unprecedented electronic control of NPG either through a rational chemical design[4] or by external means such as electrostatic gates (**Fig. 1a**).[5] Our simulations of local injection of currents in NPGs evidence the control capability of spatial current distribution with sub-nanometer precision (**Fig. 1b-c**), results which could be experimentally probed using SPM. Our most recent studies also generalize these ideas to other types of carbon nanostructures[6] and, importantly, their applicability at finite temperature. A fundamental strategy to design carbon nanodevices with built-in externally tunable electronics and spintronics is thus proposed, and should be key for future applications such as bio-chemical nanosensing and carbon nanoelectronics.

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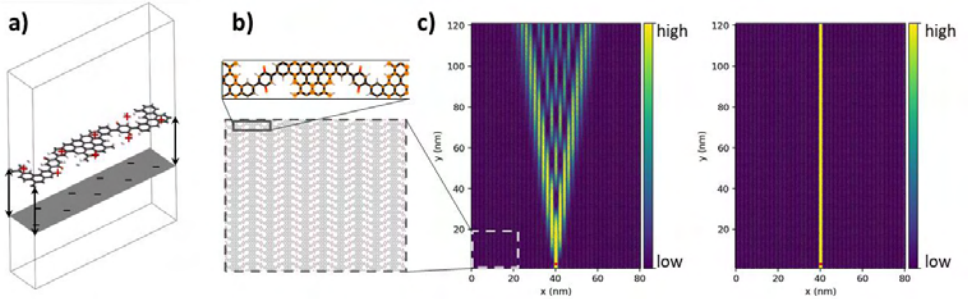

Figure 1: (**a**) Periodic unit cell of an electrostatically gated (gray plane) newly designed NPG, where GNRs are connected via aryl-quinone units. (**b**) Construction of large-scale NPG devices. (**c**) Spreading of currents (maximum magnitude in yellow) locally injected at the bottom of large-scale NPG devices (see red dot) at different applied gates (as outlined in **a**).

The effect of the linker on graphene biosensing chips' performance

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Abstract

The unique physical and chemical properties of graphene make it a promising material for biosensing applications. Here, we study the effect of the linker used to immobilize single-stranded DNA probes (ssDNA) on graphene surfaces on the performance of graphene field-effect transistors (GFET)-based biosensing chips. We use quartz crystal microbalance with dissipation (QCM-D) measurements to characterize in situ and real-time the immobilization of ssDNA and the subsequent DNA hybridization on model graphene surfaces. Like those in the graphene chips [1], the surfaces were previously biofunctionalized via heterobifunctional linkers. The GFET's transfer curves were used to characterize the biosensor chip performance.

The ssDNA immobilization kinetics and thermodynamics were investigated for all the pairings between three bifunctional linkers: 1-pyrene butyric acid succinimidyl ester (PBSE), Fluorenylmethylsuccinimidyl carbonate (FSC), and Acridine Orange (AO) succinimidyl ester—and three organic solvents (DMF, DMSO, and 10% DMF/Ethanol) [2]. Spatial orientation of the linkers and effective surface modification for ssDNA attachment was evaluated based on footprints and quantification of ssDNA surface coverage. Among the investigated linker-solvent pairs, functionalization with PBSE in DMF led to the highest ssDNA surface density of up to 1.4 × 10^{13} cm^{-2} (Fig. 1), with a 1 aM (10^{-18} M) complementary DNA limit-of-detection (LOD), and a sensitivity of 33 mV/decade (Fig. 2). In a separate experiment, probe DNA was let adsorb onto bare graphene (no linker) via π-π interaction, and the QCM-D and GFETs' transfer curves were monitored while the complementary DNA was introduced. These experiments provide an estimation of 20% to 30% of ssDNA direct adsorption on a graphene Surface functionalized with a linker, i.e., non-specifically adsorbed.
Lastly, the GFET transfer curves using different linkers were used to simulate the output of four GFET sensors mounted in a Wheatstone bridge configuration (two graphene transistors functionalized with probe DNA, two not functionalized), showing that this configuration would result in doubling the sensitivity of the biosensor (Fig. 3). Our results demonstrate the importance of understanding the functionalization phenomena at the graphene surface to achieve high ssDNA surface density functionalization to maximize the sensor response.

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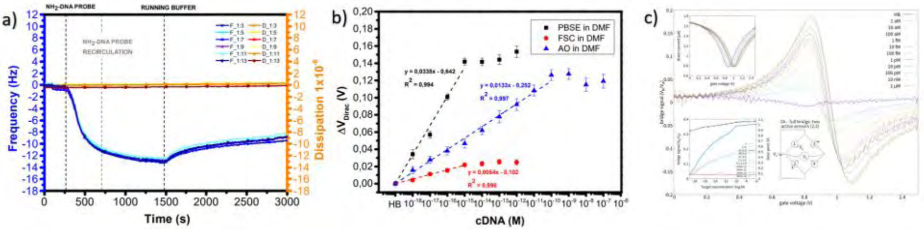

Figure 1 – (A) Measurements with quartz crystal microbalance with dissipation (QCM-D). Frequency (blue, left axis) and dissipation (orange, right axis) change vs. time response for probe immobilization with different linkers and solvents. (B) Measurements with Graphene Electrolyte-gate field effect Transistors. Calibration curve for different linkers dissolved in DMF. (C) Simulated bridge signal as a function of the applied gate voltage for different concentrations of target DNA, obtained using the measured output from 4 GFETs taken from the calibration curves of the sensor.

Progressive cluster approach to photoemission in transition metal dichalcogenides

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We present a fully atomistic approach to transition metal dichalcogenides (TMDC) angle-resolved core-level photoemission[1,2]. We calculate the fully differential cross section and Wigner time delay from the dipole-transition elements. The initial- and final-state wavefunctions are generated via a central partial-wave expansion complemented by smaller off-center auxiliary partial-wave expansions that approach B-Spline methodology [3]. Electrostatic interactions between the active electron and the rest of the cluster are taken into account through a DFT model with a LB49 exchange-correlation potential.

By comparing the cross sections and Wigner delays obtained for different model clusters we are able to dissect the underlying processes taking place as the photoelectron scatters throughout its parent system. This gradual-construction approach from smallest to largest cluster provides a reference to indicate which neighboring atoms the photoelectron is deflecting off of.

Figure 1 (left) ilustrates how we construct the clusters by adding atom perimeters respecting the group symmetry, D3h and C3v in our study cases. As an example we show the resulting WSe_2 W*4f* photoemission cross sections (middle) from model cluster W_7Se_6 and Wigner time delays (right), which will be compared to the corresponding parts from smaller or larger clusters.

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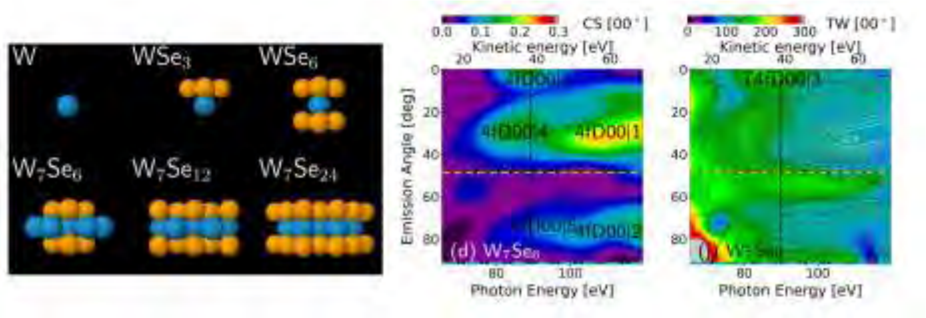

Electronic and Magnetic Properties of Organic Kagome Polymers

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Abstract:

Recent studies on carbon-based triangulene (CTN) dimers and hexamer nanostars on Au(111) surface have revealed that high spin states of adsorbed species are not totally screened by the metal and that magnetism may persist [1-2]. Based on first-principles density functional theory (DFT), we propose a promising route to control the quantum phase transition in 2D organic polymers based on CTN monomers by incorporating lightweight elements like boron or nitrogen [3-4]. Although the pure triangulene based Kagome polymer shows Mott-insulating antiferromagnetic phase, inducing organic substituants like B and N can alter the magnetic phase to ferromagnetic. Moreover, the symmetry in these types of polymers play a major role on the electronic structure, specially in controlling the band dispersion around Fermi level. Furthermore, a longer linker between the monomers can amplify the total magnetic moment along with the topological edge states. In addition, B-substituted polymers exhibit high mobility carriers while the N-substituted polymers are half-metallic where the minority spin shows mobility close to silicon. In brief, this presentation will mainly focus on different aspects to uncover collective magnetism in metal-free nanosystems. These findings may open the door for various low-dimensional organic nanomaterials based new quantum phenomena to achieve room-temperature superconductivity for applications in eco-friendly biodegradable solid-state spintronic devices.

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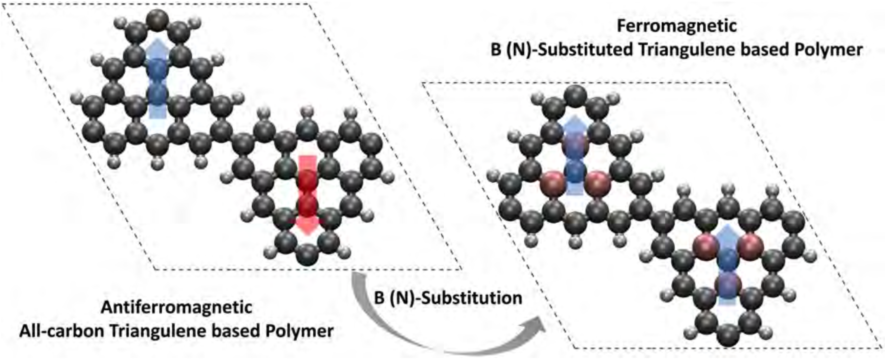

Figure 1: Tuning the magnetic phase of carbon derived Kagome polymers by B(N) substitution.

In air characterization of the mechanical properties of single bacteria based on multimode tracking of squared nanomechanical resonators

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Nanomechanical resonators have emerged as excellent tools in microbiology due to their extraordinary capability to characterize the mass and mechanical properties of a variety of microbiological entities, such as human cells, bacteria, viruses and proteins [1]. Researchers have succeeded on characterizing individual human cells in liquid environment. However, the mechanical characterization of single bacteria, viruses or proteins is usually limited to vacuum condition, being far from their intrinsic conformation.

In this work, we use a previously developed technique in order to deposit individual bacteria cells in controlled positions of squared shaped nanomechanical resonators (40µm length and width, 100 nm thickness). We simultaneously track multiple mechanical resonance frequencies of the sensor before and after the adsorption of the bacteria cells (Figure 1.a). In particular, we monitor the 1st and 2nd flexural modes, together with the 1st torsional and 1st U-shape modes. Notably, the associated mode-shapes of these modes are very different, which allows disentangling the mass and stiffness effects induced by the analytes adsorption. The method is performed in air, enabling the characterization of the bacteria properties close to their intrinsic conformation. We apply this technique for two kinds of bacteria: *Staphylococcus Epidermidis* and *Escherichia Coli* (Figure 1.b-c). We demonstrate that we obtain very accurate information about the analyte masses and their different stiffness components [2]. Importantly, accessing the different stiffness components of the bacteria allows us to determine their shape, which is essential to univocally identify them [3].

In the near future, we plan to extend this technique for liquid operation, which will strongly impact the biomedicine and biophysics fields. For example, to monitor in real time the bacteria properties while applying antibiotics, notably, at the single level, may allow to in-situ study their responses, providing a very powerful tool to delve into antimicrobial resistance emergence. Moreover, the developed technique may find applications for many other microbiological analytes, going from human cells to viruses.

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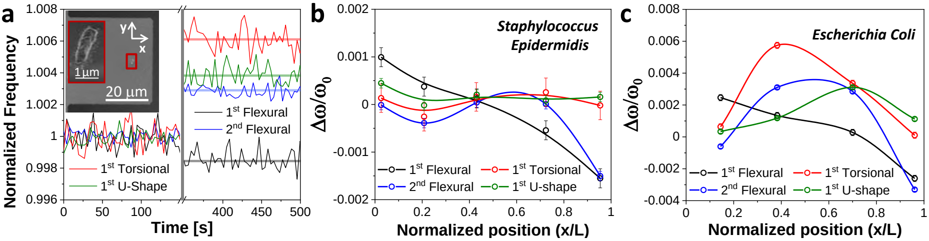

Figure 1.a. Normalized frequencies (ω/ω_0) of the first four mechanical modes of the sensor (1st flexural, 1st torsional, 2nd flexural and 1st U-shape) before and after the adsorption of an *Escherichia Coli* cell. Insets show scanning electron microscope images of the nanomechanical squared resonator (40µm length and width, 100 nm thickness) with the adsorbed *Escherichia Coli* cell. Solid lines indicate the averaged normalized frequencies after the bacterium adsorption. **b-c.** Relative frequency shift of the first four mechanical modes of the sensors induced by the adsorption of *Staphylococcus Epidermidis* and *Escherichia Coli* cells, respectively, versus the normalized longitudinal position (x-axis). All the cells are adsorbed on the sensors central position respect to the y-axis. Solid lines are guides to the eye.

Piezoelectricity in monolayer hexagonal boron nitride

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Two-dimensional (2D) hexagonal boron nitride (hBN) is a wide-bandgap van der Waals crystal with a unique combination of properties [1]. Furthermore, in recent years hBN crystals have become the material of choice for encapsulating other 2D crystals in a variety of technological applications [2]. Monolayer hBN was predicted to exhibit piezoelectric properties because it has no center of symmetry, however experimental evidence was lacking. In this work, we used AC Bias electrostatic force microscopy (EFM) to observe this effect [3] as a strain-induced change in the local electric field around bubbles and creases, in agreement with theoretical calculations. No piezoelectricity was found in bilayer and bulk hBN, where the center of symmetry is restored. Our results add piezoelectricity to the known properties of monolayer hBN, which makes it a desirable candidate for novel electromechanical and stretchable optoelectronic devices, and pave a way to control the local electric field and carrier concentration in van der Waals heterostructures via strain. The experimental approach used here also shows a way to investigate the piezoelectric properties of other materials on the nanoscale by using electrostatic scanning probe techniques.

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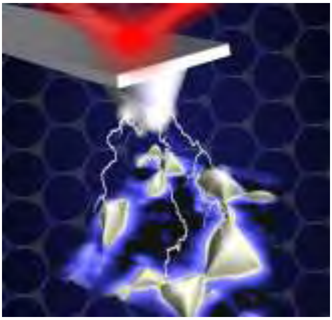

Figure 1: strain-induced change in the local electric field observed around bubbles in monolayer hBN

Truncated TDDFT Approach for the Calculation of Exciton Binding Energies in Solids

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The calculation of the excitonic effects in solids is a crucial step towards the prediction of the optical properties of new materials. The Bethe-Salpeter equation (BSE) is the standard method to compute excitations in solids, but its computational cost limits its applicability. In the last years, Time Dependent Density Functional Theory (TDDFT) has shown to be a low-cost alternative to the BSE that yields reasonable excitations[1]. By solving the Casida equation with exchange-correlation kernels that include the long-range Coulomb interaction, some excitonic features can be obtained. However, these results are critically dependent on the transition dipole moment, which is an ill-defined magnitude in solids[2] (see Fig. 1). Recently, a promising hybrid approach has been proposed by Sun et al.[3], which includes a fraction of the screened exact exchange (SXX) in conjunction with TDDFT.

In this work, we explicitly treat the singularity of the SXX kernel by truncating the Coulomb interaction in the Wigner-Seitz supercells of the compounds under analysis[4]. This way, we get a well defined, material dependent term that can be related with the exciton radius. Our preliminary results show that this approach can be used to get exciton binding energies in good agreement with experiments at the computational cost of TDDFT, which could be crucial for future investigations.

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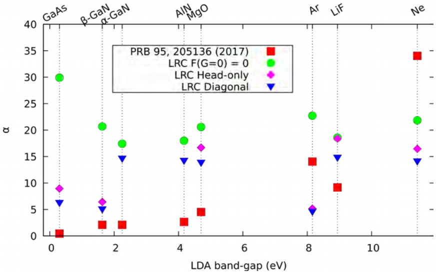

Figure 1: Scaling parameter of the Coulomb interaction needed to reproduce the experimental exciton binding energy with different TDDFT kernels.

Topological confinement and geometry dependence in bilayer graphene

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Abstract

We investigate in this work a study of topological confinement of electrons in bilayer graphene material. We discuss the case of topological loops with different shapes. These loops are created by lateral gates acting via gap inversion on the two graphene sheets. We consider loops of higher to lower symmetry (circle, square, rectangle, and irregular polygon). For a small-size loop, we found that the spectrum depends on the loop shape. By applying a perpendicular magnetic field, the spectrum shows valley splitting of the states and the emergence of persistent currents.

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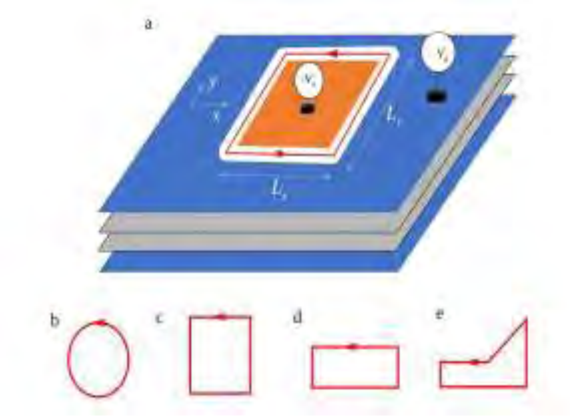

Figure 1: a) Scheme of a topological loop showing the BLG sheets (gray) and lateral gates with the applied gate potentials ±Va (orange and blue, respectively). Two identical lower gates, hidden behind the lower graphene sheet, have the opposite potentials of the corresponding top gates. The white 1D region between orange and blue gates hosts the topological loop state on the graphene sheets, with counterpropagation for the two valleys. A red arrow is indicating the circulation for only one of the two valleys. (b)–(e) Loop shapes considered in this work, from highest to lowest symmetry: circle, square, rectangle and irregular polygon.

Exploiting orientation of anisotropic nanoparticles in topological plasmonic arrays

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Abstract

In the limit of small size, single metallic nanoparticles behave like electric dipoles. An array of metallic nanospheres with alternate distances is then a plasmonic analogue of the SSH model [1]. However, nanoparticles have features that fundamental particles lack, e.g. dimensions or geometrical form, which can be exploited in plasmonics to explore topology beyond condensed matter. When particles are anisotropic, surface plasmon resonances occur at different frequencies depending on the axis. Then, if the anisotropy is significant, near the plasmonic resonance in one axis, the dipole is projected along that same direction [2]. Here we show that this projection can be used to tune the coupling between the nanoparticles in an array, allowing to open topological gaps without alternating distances. As an example of the potential of the use of anisotropy for topology, we study 1D chains of prolate spheroidal silver nanoparticles.

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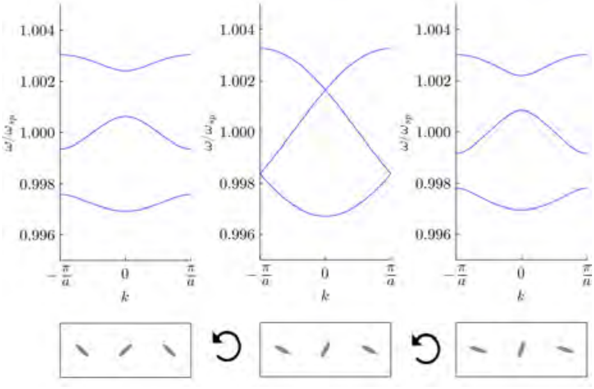

Figure 1: Bands for different orientations of the nanoparticles: By rotating nanoparticles in the unit cell, we can open topological gaps.

Nanostructured bismuth telluride electrochemically grown inside flexible templates

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In this work, we present different nano-structures of bismuth telluride based on scalable and low cost fabrication techniques. The objective is to improve the thermoelectric performance of this material grown by electrochemical deposition, and then use these nanostructures to develop efficient flexible thermoelectric generators (TEGs) which will allow the conversion of wasted heat around room temperature into usable electrical energy.

The main advantage of nanostructures over thin films or bulk is that they should increase the thermoelectric performance of the bismuth telluride (which is the most used thermoelectric material for room temperature appilcations) by lowering its thermal conductivity. This has been already proved for 3D interconnected nanowire networks of bismuth telluride [1]. In that work, we showed that both the increasing of the surface to volume ratio and the influence of the nanostructure in the the phonon scattering phenomena are the main responsibles of the improvement, but the templates used in that case were made of non-flexible alumina. Here, we will use two different flexible commercial templates to obtain nanostructured thermoelectric materials by template-assisted electrochemical deposition of bismuth telluride: polyester membranes (obtaining an intrincate 3D nanostructure) and cellulose membranes (obtaining a highly porous structure). As it was previously done with the growth of bismuth telluride inside alumina templates [2], the nanostructured bismuth telluride grown inside the flexible templates will be then characterized to optimize the fabricartion parameters to obtain highly oriented, stoichiometric material in such nanostructures.

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An Automated System for Strain Engineering and Straintronics of Single-Layer MoS_2

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Strain engineering in 2D materials has received extensive attention. Research in the field has already demonstrated piezoelectricity[1], bandgap tuning[2] and enhancement of thermoelectric figures of merit[3]. However, typical straining setups consist of manual micromanipulators[4] and have measurement limitations in long time and short strain intervals. The experimental results also suffer from accuracy because of these limitations. Therefore, we constructed a new setup with a motorized vertical translation stage and controlled it by PC. After calibration, the lowest strain value has been found as ~10^{-6} %. Then, we have tested the setup by performing differential reflectance, photoluminescence, Raman spectroscopy, IV measurement and photoresponsivity on monolayer MoS_2 with several cycles. Gauge factors calculated in each measurement were found comparable with the previous results in literature. The setup can be a good candidate for straining experiments in a long time in order to discover their performance optically and electrically. Moreover, the measurements demonstrate lower strain interval and more repeatable cycles can lead to higher accuracy as well.

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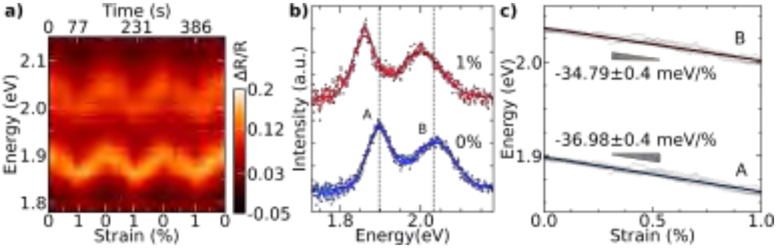

Figures

Electronic properties of a 1H/1T/2H-TaS2 polymorphic vdW heterostructure

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1H/1T-TaS2 heterostructures were first studied in 4Hb-TaS2 crystals in the decade of the 90s [1,2]. More recently, in 1T-TaS2 crystals and HOPG, an increase in the superconducting (SC) critical temperature has been reported [3,4]. In this work we study a 1H/1T heterostructure in a 2H-TaS2 crystal and, contrary to previous publications, no increase in the SC critical temperature is found. Instead, a non-SC gap appears in the local density of states of the 1H/1T heterostructure (see green dotted lines in figure 1C), possibly hindering the expected boost in critical temperature. The variation with temperature and magnetic field together with the shape of the gap allow us to trace back its origin to the long-range interaction between electrons close to the Fermi level [5]. Another intriguing property of this material is the transparency of the metallic 1H layer to the CDW of the 1T layer underneath [1,2], that results in strongly bias dependent STM images where both CDWs can be detected simultaneously (see panels a and b of figure 1). Our STS data (panel c) allow us to explain this effect as a direct tunneling process to the upper Hubbard sub-band of the 1T layer underneath (see purple arrow in figure 1C).

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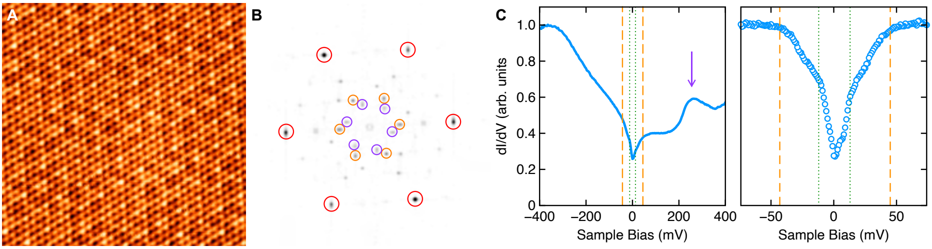

Figure 1: **A:** Atomic resolution STM image of 1H/1T/2H TaS2 recorded at 1.2 K. Image parameters: V=100 mV, I=300 pA, size: 10 x 10 nm^2. **B:** FFT map corresponding to the image of panel A. Red, orange and purple circles mark the 1st order spots of the atomic lattice, 1H CDW and 1T CDW respectively. **C:** STS spectra recorded over 1H/1T/2H TaS2 at 1.2 K. Orange dashed lines mark the onset of the pseudo-gap associated to the 1H CDW, and the purple arrow points to the upper Hubbard sub-band from the 1T layer underneath. Right panel has been background-subtracted.

The influence of pH during the adsorption of catechols on the magnetic properties of superparamagnetic iron oxide nanoparticles

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In the past 20 years, superparamagnetic iron oxide nanoparticles (SPIONs) have been widely used in biomedical applications as MRI contrasting agents or as a means of transportation of drugs for drug delivery [1-4]. The surface of SPIONs needs to be tuned to prevent dissolution and promote the biding of specific molecules. Amongst a variety of functional molecules catechols are commonly used due to their small size, stable bonding through chelate bonds and variety of functionalization groups. Catechols are non-innocent ligands and they influence the magnetic properties of SPIONs, namely, they increase the saturated magnetization [1-3,5,6].

In this study, we have found that the successful bonding of catechols to the surface of SPIONs increases their saturation magnetization by more than 10%. The increase of magnetization depends on the pH at which the adsorption takes place. This is strongly related to the pKa values of deprotonations of OH groups in catechols. As long as the pH of adsorption is low enough to keep at least one of the OH groups protonated, we can observe significant increases in the magnetization of SPIONs. Once all the OH groups are deprotonated, the chelate bonding is not formed and the magnetization is not affected. The surface of the samples was characterized using several analytical techniques including XPS, TEM, EELS and electrochemical measurements. Additionally, theoretical modelling was implemented to determine the influence of catechol bonding on magnetic properties.

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Analysis of the magnetic interactions in arrays of FeNi nanowires by means of angular hysteresis loops and FORC measurements

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Compositional variation in magnetic nanowires (NWs) through controlled growth conditions allows to tailor their magnetic properties [1], which are affected by different factors such as geometry, composition or magnetic interactions between NWs. Herein, arrays of FeNi NWs have been electrodeposited into anodized aluminium oxide (AAO) membranes (Fig. 1a). Chemical composition analysis of the NWs showed anmolaous co-deposition, where Fe deposits in ratios higher than its electrolyte molar fractions under different trends. These effects were explained within a modified Bocris-Drazic-Despic (BDD) model [2].
Coercivities (H_c) ranging from 0.2 kOe to 1.0 kOe were obtained (Fig. 1b), observing an increase in H_c for a diminished Fe concentration. The angular hysteresis loops measurements allowed to determine that the magnetization reversal mechanisms is dominated by transverse domain wall reversal, and indicated the decrease in the magnetostatic interactions between NWs as the source of the rise in H_c. First-order reversal curve (FORC) analysis highlighted the limited role of the magnetic interactions in the arrays (Fig. 1c), except for $Fe_{0.80}Ni_{0.20}$ NWs which showed the typical FORC diagram for magnetically interacting NWs. FORC diagrams showed higher intensity at around H_c = 1 kOe, with weakening intensity for an increased Fe content due to the enhanced interactions.
This work shows the possibility of tailoring the magnetic properties of FeNi NWs by tuning the electrochemical parameters and, thus, their composition and crystallographic structure. This approach is of interest in applications such as magnetic recording and sensing devices, and opens the path to exploring the formation of ordered phases with outstanding permanent magnet properties (e.g. $L1_0$-FeNi phase [3]).

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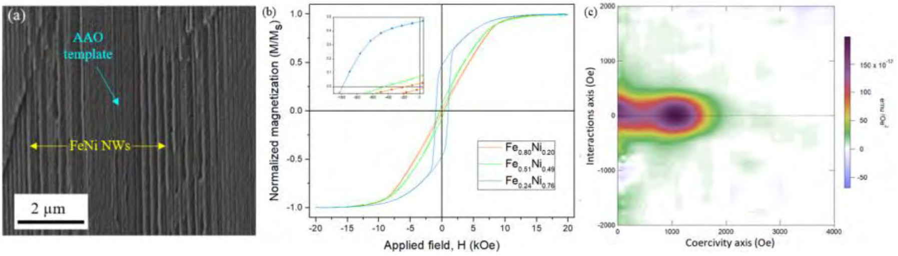

Figure 1: (a) FeNi NWs in an AAO template; (b) room temperature hysteresis loops measured for arrays of FeNi NWs with different compositions; and (c) FORC diagram obtained for an array of $Fe_{0.51}Ni_{0.49}$ NWs.

Acknowledgments

Authors acknowledge financial support from EU M-ERA.NET and MICINN through the projects *COSMAG* (PCI2020-112143) and *NEXUS* (PID2020-11521RB-C21). A.J.C.-H. acknowledges support from “La Caixa” Foundation (ID 100010434) through the Doctoral INPhINIT Incoming program (LCF/BQ/DI20/1178002). E.M.P. acknowledges support from AEI through the Juan de la Cierva – Incorporación program (IJC2020-043011-I/MCIN/AEI/10.13039/501100011033) and EU by NextGenerationEU/PRTR.

Gallium nanoparticles for improved III-V solar cells

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Abstract

In the last decade, third generation solar cells have progressed very strongly in efficiency, which is a key metric in the development of photovoltaic systems to reduce the cost of electricity per kilowatt-hour. The short-circuit current (J_{SC}) and the open-circuit voltage (V_{OC}) of the solar cell are the two main factors that should be considered to have an optimized efficiency. Some materials show moderate J_{SC} values that indicate that better light management must be applied to improve the solar cell. This includes better coupling and trapping of light above the cell and reduction of light absorption in inactive regions of the cell [1]. In this work, we report on the improved performance of GaAs solar cells via light scattering from gallium nanoparticles (Ga NPs) deposited atop the devices. After minimal nanoparticle size optimization to tune its plasmonic effect, J_{SC} derived from external quantum efficiency measurements is increased around 18%, revealing a higher light collection. We also demonstrate a similar efficiency enhancement in III-V solar cells made of GaAsSb/GaAsN superlattices. This structure [2] is designed to form the lattice-matched 1.0–1.15 eV subcell that would allow the implementation of the optimum monolithic 3 and 4-junction solar cell structure. Theoretical calculations made with COMSOL Multiphysics software and detailed reflectance spectroscopy measurements reveal the role of the NP size and plasmonic effect in each case. Compared to the complex antireflective coatings used in the literature, this work shows an easier method that can be implemented insitu after growth of the solar cell.

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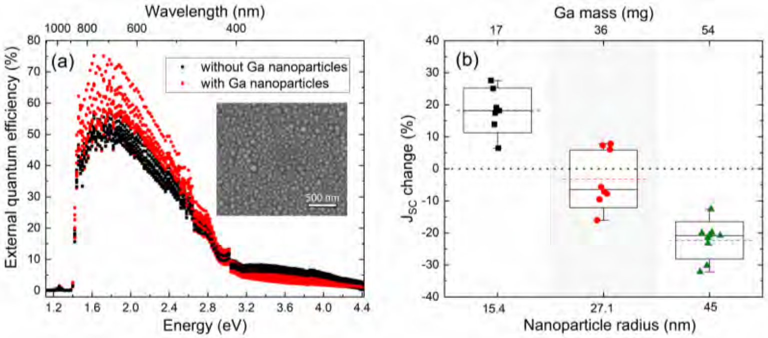

Figure 1: (a) External quantum efficiency (EQE) of different GaAs solar cells before and after Ga NPs deposition. (b) Short-circuit density current (J_{SC}) change (%) for different NPs radius atop the solar cells.

Bismuth telluride thin films with intrinsic nanostructured morphology

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We present a straightforward way of obtaining nanostructured bismuth telluride by electrochemical growth in the presence of certain additives. A conventional three-electrode cell, with reference electrode Ag/AgCl (saturated KCl), platinum counter electrode, and working electrode composed of silicon coated with chromium and gold, was used. The films were grown from a nitric acid bath [1] with sodium lignosulfonate added to the electrolyte, as we had already studied in a previous work to improve the morphology and crystallographic orientation of bismuth telluride thin films [2].

As a result of the growth conditions, a morphology of highly oriented nanoplatelets, with the c-axis oriented parallel to the surface of the substrate. These nanoplatelets present one dimension much smaller than the two others, in the order of 10 nm, while the other dimensions can be in the order of the microns. It is remarkable that these nanostructures grow without the need of a template, and that they present a high homogeneity in areas of square centimeters.

Then, these thin films have been optimized to obtain stoichiometric bismuth telluride films, with a defined crystallographic orientation. The best films have been characterized from a thermoelectric point of view, given that it is expected that the transport properties should be affected by the low dimension of the structure and as a result, the whole thermoelectric efficiency should be increased [3]. To this end, a technique to detach the nanostructured films from the working electrode has been developed, in order to avoid the influence of the conductive layers in the measurements. In such a way, we are able to measure the transport properties along the length of the nanostructured film. We will present a first characterization of the electrical conductivity, Seebeck coefficient and thermal conductivity of such nanostructures.

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NanoGPS Suite: New advanced solution for correlative optical & electron microscopy

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A single instrument or technique can’t give you the complete information regarding a sample. When sample is a macro sample, splitting the specimen in several pieces in case of destructive analysis or reusing the same sample if the analysis is not destructive usually solve the problem.

In case of 2D sample problem can be more complex. Marking manually the sample with a pencil or other medium is an easy way but not always effective when moving the sample from one instrument to another. Sometime within the portfolio of a manufacturer some proprietary solutions do exist but usually limited to that specific manufacturer and not all characterization techniques maybe available.

Hyphenated instruments can be another solution but usually when an instrument becomes more complex, ease of use is lost and sometimes compromises are done making that some specific features are lost.

Today world is connected, and my daughter could not imagine how to meet with friends at a place without sharing her position by WhatsApp. That the thought that some scientist had at Horiba when they came to the development of Nano-GPS: We want to easily share the points of interest of a sample at Nano scale, and share that position easily on different instruments platform from optical microscope, Raman microscope, AFM microscope to electron microscope SEM, FIB, HIM, #XGT X-Ray microscope…

Integrating and treating these nice data was the next mandatory step to have a solution that could be accepted by the scientist. We choose to develop #graphXY software suite with the help of #Digital Surf using their experience on #Mountains software considered as a standard by part of the community. #graphXY allow an easy integration of the different images to generate impressive #correlative reports and papers

HORIBA took some time to develop test and validate the concept on different platforms but today product launch is ready. Please don’t hesitate to get and test your first nanoGPS tags!

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Novel 1D silicon nanoribbons

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Abstract

One-dimensional atom-thin Si nanoribbons (1D SiNRs) could be key elements in future high performance devices. Here, we will compare different SiNRs grown *in situ* under ultra-high vacuum on two noble metal substrates with practically the same lattice parameter, namely, Au(110) and Ag(110).

In particular we will address the role of the initial missing row (MR) reconstruction formed spontaneously on the clean bare Au(110)(2×1) template. This reconstruction is washed out upon forming firstly a two-dimensional surface alloy and is followed by the growth of a variety of massively parallel 1D SiNRs aligned along the Au(110) [1-10] direction observed and analysed in high-resolution Scanning Tunneling Microscopy and synchrotron radiation PhotoElectron Spectroscopy, respectively [1].

Instead, the MR reconstruction of the Ag(110) surface is promoted by the adsorption of silicon. The atomically precise SiNRs residing there comprise solely unique alternating Si pentagons in either single strands, 0.8 nm in width upon room temperature preparation, or 1.6 nm wide associated double strands after annealing or preparation at 200°C [2]. They can form by self-assembly a highly perfect (5×2) grating covering the entire surface. It is the first pure pentagonal phase ever found for silicon low-dimensional structures, i.e., a 1D form of pentasilicene. These unique SiNRs with Dirac-like signatures can be detached from the substrate surface by the STM tip [3].

Possible applications of this taxonomy of SiNRs, typically as 1D channels in future transistors, will be discussed.

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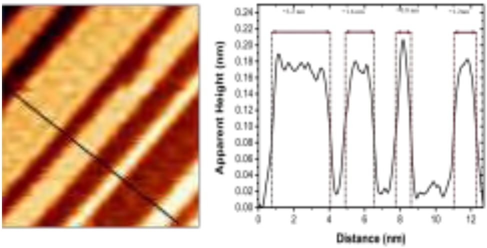

Silicon nanoribbons grown within a 2D surface alloy on Au(110)

Collective modes of superconducting monolayer NbSe2

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While bulk 2H-NbSe2 is generally accepted to be a conventional superconductor, several unconventional features of the superconducting state have been reported in the monolayer limit, including the breaking of threefold symmetry in magnetotransport and anomalously large in-plane critical fields. In this talk, I will first present another unconventional feature: the existence of satellite peaks in the STM spectra of NbSe2 monolayers which exist only in the superconducting state [1]. After discussing potential candidate explanations, I will propose a scenario of competing pairing between s-wave and subleading f-wave triplet channels to address the different experimental observations. In this scenario, the STM peaks can be interpreted as a superconducting collective Leggett mode.

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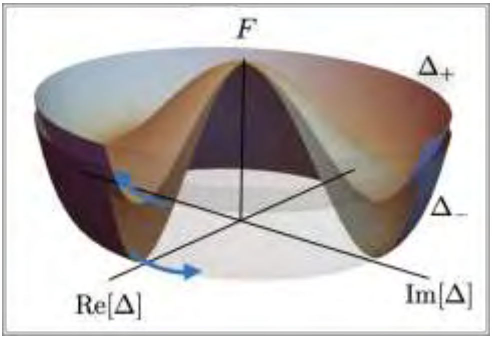

Figure 1: Relative phase oscillations of two pairing fields give rise to a Leggett collective mode. From Ref. [1]

Mechanically-induced spin-polarization in non-magnetic metal nanocontacts

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Symmetry breaking can lead to exotic and potentially technologically useful phenomena, even in materials that are non-magnetic. For example, the Shockley surface state manifests on an exposed surface of Au111 as a result of Rashba spin-orbit (SO) splitting [1]. Other recent examples are the non-trivial edge and surface states that manifest in strong-SO topological insulators [2]. More recently, and also of great interest, is the socalled chirality-induced spin selectivity (CISS) effect in molecular nanojunctions containing chiral organic molecules [3]. The CISS effect has been attributed to symmetry breaking at the metal-molecule interface [4]. In this work, using a Gaussian-type orbital (GTO) density functional theory (DFT) approach [5] to obtain SO-corrected bands (see Fig 1), allowing the efficient modelling of complex nano-structures which are intractable by other methods, we show that strong spin-polarization can manifest even in non-magnetic metal nanocontacts where centro-symmetry is broken by simple mechanical rotation (see Fig. 2). Our results are likely to form the basis for insights into more complex systems, such as the molecular nanojunctions in which the CISS effect is important.

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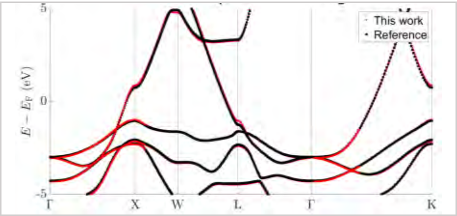

Figure 1: Comparison of SO-corrected bands about the Fermi level obtained using our method (red) and a reference method (black) for face-centred cubic Au.

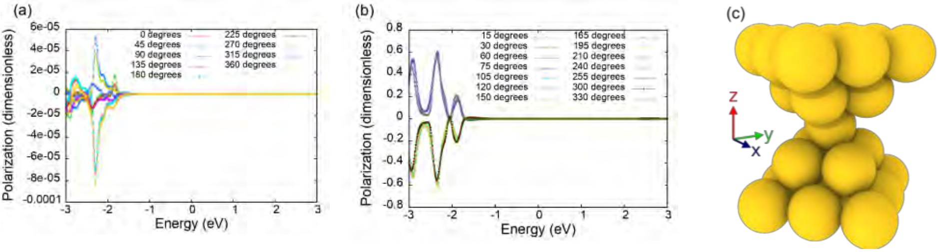

Figure 2: Spin-polarization at (a) highly symmetric and (b) unsymmetric angles as one end of a simple Au9-Au4-Au-Au4-Au9 nanocontact (c) is rotated about the *z*-axis. In (c), the top half has been rotated by 45° with respect to the bottom.

Metamaterials based on nanoporous anodic aluminium oxide for passive radiative cooling applications

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The development of metamaterials with tunable photonic properties is followed by interesting possibilities for energy saving and harvesting, among others. A significant reduction in energy demand will be achieved when passive radiative cooler technology meets low-cost, easy-scalable to industry metamaterials. The crucial optical requirements are both high reflectance of the solar radiation and a strong thermal radiation. Since cooling was demonstrated using nanoporous anodic aluminium oxide (AAO) membranes[1], these nanostructures have been involved as the principal material as well as useful templates for achieving passive radiative cooling. A detailed analysis about AAO-Al films, including: fabrication by two-step anodization process in different electrolytes (phosphoric acid, oxalic acid, sulphuric acid and ethylene glycol containing sulphuric acid); morphological characterisation (SEM and AFM) of pore diameter, interepore distance, pore's arrangement order grade, porosity, and different alumina thickness; and the impact of these parametes in the optical response from UV-Vis to mid-IR. The solar reflectance and the thermal emission have been characterised, achiving UV-Vis to near-IR reflectivity above 80%[2], and an IR emissivity around 90% up to 8 µm. Aditionally, AAO-Al films' cooling performance have been experimentally studied during several day-night cycles.

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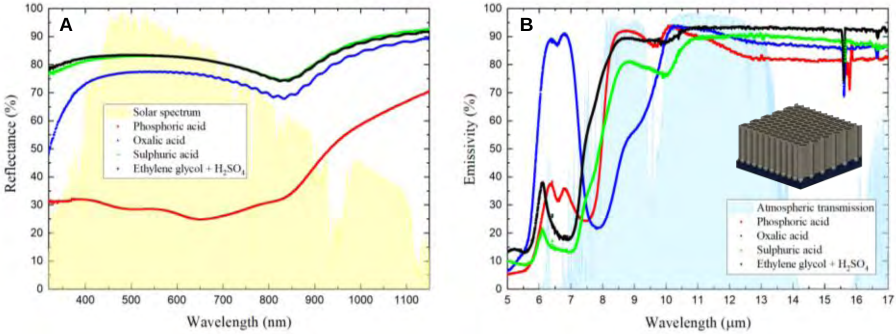

Figure 1: (A) AAO-Al films' reflectance from UV-Vis to near IR, over the solar irradiance spectrum. (B) AAO-Al films' IR emissivity above the atmospheric transmission spectrum. Nanostructure scheme is shown in the inset.

Improving Electrical Conductivity of Films of Interconnected Graphite Flakes by Laser Induced Annealing

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In the last years, van der Waals materials have been integrated into the catalog of electronic materials employed in printed electronics. The colloidal suspension of flakes of these materials as prepared as inks and films of them are deposited by printing techniques like inkjet printing, brush coating, or spraying, among others. These films, formed by a network of interconnected platelets, tend to contain water, solvents, or surfactants used to stabilize the colloidal suspensión, trapped between the platelets severely degrading the electrical performance of the resulting films [1,2]. Strategies to remove these interstitial molecules are therefore critical to achieving optimal properties. To remove contamination, several methods have been reported. e.g thermal annealing, vacuum annealing, etc. [3,4,5]. However, annealing at high temperatures causes severe damage and is not suitable for paper-based and plastic-based electronics.

Herein commercial laser engraving system is introduced that can improve the electrical conductivity of graphite films without damaging the paper or other flexible substrate. The results were evaluated by resistance measurements, and it was observed that the laser-induced annealing improved the electrical conductivity of films containing interstitial molecules. This approach provides a route to cleaning the surface with the advantages of a fast, easy, and low-energy consumption process.

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Nanoscience and Covid-19: MD simulations of the interaction of the SARS-CoV-2 virus with materials and chemical agents

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The novel coronavirus SARS-CoV-2 emerged in December 2019 as a human pathogen that causes the COVID-19 pandemic. From the point of view of NanoScience, this virus is an organic nanoparticle with a diameter of ~90 nm made by a vesicle-like envelope of proteins and lipids encapsulating the viral genetic material. The virion particle has a large protruding spike S glycoprotein (~24 nm long) that covers the viral particle and give its crown-like characteristic appearance (hence the latin name "corona"). During these two years of pandemic, a wealth of structural information about the viral nanoparticle has been accumulating, including detailed 3D images of the envelope, protein structures with atomistic-resolution and many other molecular and supramolecular details. In our group, we have been employing this information in order to develop models of the virus and its interaction with materials and chemicals, using molecular dynamics (atomistic and coarse-grain) simulation techniques. This is a topic of fundamental importance, given its role in virus transmission (filters, face masks, possible surface contamination,…) and disinfection (use of soap or alcoholic hydrogel, air cleaning devices,…).

First, we have considered the interaction of materials with the virus. Since this interaction is mediated by the spike S glycoprotein that covers the viral particle, we have considered the interaction of S (protruding from a virion) with surfaces of different materials of interest. We have considered common materials such as cellulose, graphite and polystyrene. We found that graphite substantially deforms the S protein [1]. On the contrary, the S protein adsorbs over cellulose with little deformation, by forming hydrogen bonds between its receptor binding domain and adjacent residues and the cellulose (some of them mediated by hydration) [1]. In the case of polystyrene, we found strong interaction of S with that material either with the receptor binding domain of S or the sugars (glycans) covering S, depending on the S conformation (open or closed state) [3]. Ongoing investigations of the interaction of S with metals (as included in virucidal materials in the form of nanoparticles for example) are under way. We have also studied the interaction with human skin. We found a substantial difference depending on whether the skin is covered or not by sebum. S protein has little interaction with the sebum covering certain regions of the skin but it is able to adsorb by hydrogen bonds with lipids exposed in the skin in absence of sebum.

Concerning the interaction with chemicals [3], MD simulations of a coarse-grain model of the virus and surfactants show that the disinfection action of soap may occur mostly by blocking the S protein instead of disrupting the envelope membrane. Atomistic MD simulations of the envelope in contact with ROS species show that OH* radicals are able to penetrate into the hydrophobic region of the envelope mainly in protein-lipid contacts, thus being able to disrupt the viral envelope by oxidation and suggesting an effective method for ambient disinfection.

This work was supported by the Spanish Ministry of Science and Innovation through grants RTI2018-096273-B-I00 and CEX2019-000917-S and the European Union Horizon 2020 research programme under MSCA COFUND grant agreement 6655919 (DCM) and MSCA-IF agreement 101026158 (MS). This work was partially funded by a R+D agreement with Benseny SAU company. We thank CESGA and BSC-RES for computer time and technical support at Finisterrae and MinoTauro supercomputers, respectively.

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Synthesis and Applications of Group 11-Based Ternary Chalcogenide Nanocrystals with Tunable Morphology and Composition

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The optimization of a material functionality requires both the rational design and precise engineering of its structural and chemical parameters. [1] Colloidal chemistry is an excellent synthetic choice for the synthesis of homogeneous and compositionally complex novel nanostructured systems with potential application in several fields. [2] We have exploited here several surfactant-assisted synthetic strategies in order to chemically transform our starting silver or copper chalcogenide nanocrystals into compositionally more complex nanostructured systems, such as hybrid and ternary I-I-VI semiconductor nanocrystals with different stoichiometries. Our results indicate the formation of new ternary materials, both with stoichiometric and non-stoichiometric compositions. Considering the complex chemical distribution of the species in the materials, the use of advanced atomic-resolution electron microscopy techniques was key for their appropriate characterization and elucidation of formation mechanisms. The work is complemented with the assessment of their potential as active materials for energy conversion devices and as contrast agents in clinical diagnosis.

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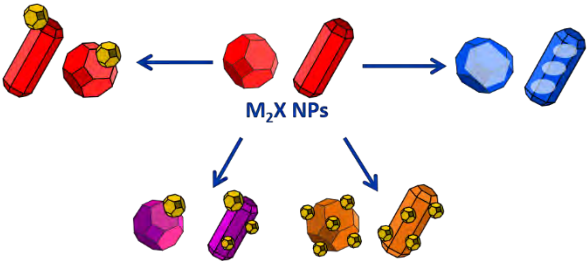

Figure 1: Chemical transformation of binary chalcogenide nanostructured materials into more complex noble metal-based chalcogenide systems with a ternary or hybrid composition. (M stands from Ag or Cu while X represents S or Se)

Toxicity Assessment of a Panel of Nanomaterials in Placental Barrier BeWo b30 Cells

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Metal nanoparticles (M-NP), inorganic non-metallic and carbon-based nanomaterials (CBM) are among the categories of nanomaterials (NM) of largest market volume [1]. The increasing number of products containing NM has raised serious concerns regarding their environmental and human safety. Biological barriers are important lines of defence to xenobiotics, thus expected targets for NM. One aspect that has been poorly addressed is the impact of NM on placental development and function. The present study aimed at evaluating the toxicity of NM of industrial, consumer and biomedical relevance in human BeWo clone b30 epithelial cells, a widely used model of placental trophoblastic cells.

BeWo b30 cells were exposed for 24 h to varied concentrations of NM of different chemical composition [Au, Ag, TiO2, SiO2 and graphene oxide (nano_GO)], primary size (10, 30 and 60 nm Au- and AgNP), capping (citrate- and PEGylated AuNP) and crystal structure (TiO2 NP rutile and anatase forms). In vitro cytotoxicity was assessed by determining changes in cell morphology, metabolic activity, plasma membrane integrity, intracellular reactive oxygen species and ATP levels. Genotoxicity (DNA strand breaks and oxidative damage) was also assessed.

No evident changes in cell morphology were observed after exposure to any tested NM. Overall, NM can be ranked for cytotoxicity as AgNP > nano_GO > AuNP ~TiO2 NP ~ SiO2 NP, being the effects more visible at higher concentrations. Regarding M-NP, the role of the size in the cytotoxic-induced effects was more evident for AgNP than for AuNP, with the smaller NP inducing more cytotoxicity in BeWo b30 cells. PEG capping was an effective capping agent for preventing the cytotoxic effects that were visible in cells exposed to the tested citrate-capped AuNP. No significant differences between rutile-anatase and anatase TiO2 NP-induced cytotoxicity were observed. Exposure to AgNP and nano_GO significantly increased ROS levels of the exposed cells suggesting that oxidative stress is a possible mechanism underlying their cytotoxicity in BeWo b30 cells. All tested NM significantly increased intracellular ATP levels compared to control cells, except for 10 nm AuNP. No significant changes in both DNA strand-breaks levels and DNA oxidative damage were detected for all tested NM.

Our findings alert for the potential risks associated with human placental exposure to NM, where the physicochemical properties are important drivers of toxicity. Additional research is needed for a deeper understanding of NM impact on human placental barrier and to unravel the properties responsible for NM-mediated toxicity, and thus support regulatory decisions that protect consumers and ultimately assist in the development of safer NM.

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Acknowledgments

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Quantum-mechanical simulations of hydrogen isotopic separation by graphyne-based membranes

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Deuterium and trititum constitute relevant substances for many scientific and industrial applications. However, they cannot be easily separated from a mixture with H_2, the most abundant hydrogen isotope, as standard methods are based on chemical properties, which are similar for isotopes. For this purpose, in this study [1], we have employed a quantum-mechanical method that takes into account mass-dependent effects. Graphdiyne, a recently synthesized porous derivative of graphene [2], offers a promising opportunity to enhance these effects, as its subnanometric pores enable a confinement of the hydrogen molecules when travelling through them. In our simulations the molecules have been treated as pseudoatoms and their interaction with the membrane is represented by an improved Lennard-Jones force field [3]. By performing three-dimensional time-dependent wavepacket propagations [4], we have obtained the transmission probability of each isotope, which in turn has been used to compute the permeances at different temperatures. Finally, we have calculated the selectivity of deuterium and tritium over hydrogen (shown in Figure 1) as the quotient of their permeances: It is seen that the selectivities (favoring the heavier isotopes) increase as temperature decreases until reaching a maximum value. The maximum is a result of a compromise between zero point energy and tunnelling effects, which benefit the heavier and lighter species, respectively. These results are promising for efficient deuterium and tritium separation from hydrogen.

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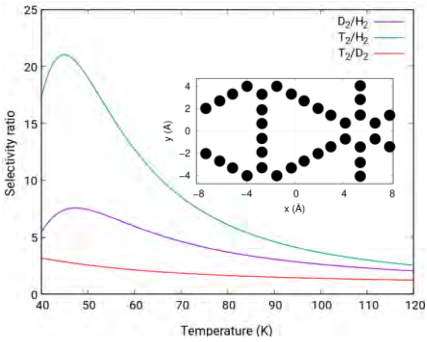

Figure 1: Selectivity as a function of temperature, inset shows the graphdiyne unit cell

Optomechanical detection of single bacterium mechanical modes

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Low-frequency phonon modes of biological particles such as proteins, viruses and bacteria involve coherent structural vibrations at frequencies in the THz and GHz domains (Figure 1.A). These modes carry information on its structure and mechanical properties that play a pivotal role in many relevant biological processes. Despite the rapid advances of optical spectroscopy techniques, detection of low-frequency phonons of single bioparticles has remained elusive. Here we harness a particular regime in the physics of mechanical resonator sensing that serves for detecting them. By depositing single bacterium on ultra-high frequency optomechanical disk resonators, we demonstrate that the vibration modes of the disk and bacterium hybridize when their associated frequencies are similar (Figure 2.A). A general theoretical framework is developed to describe the different regimes that can be found when an analyte adsorbs on a mechanical resonant sensor. Our model allows retrieving the mechanical frequencies and losses of the bacterium modes. This work opens the door for a new class of vibrational spectrometry based on high frequency mechanical resonators with the unique capability to obtain information on single biological entities [1].

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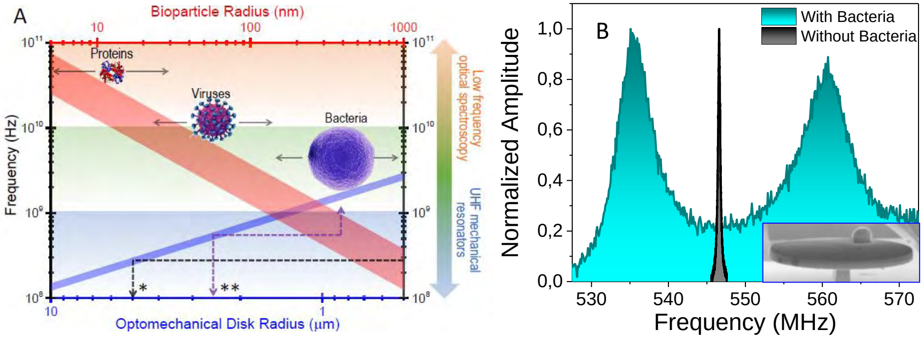

Figure 1: A. Frequency of the radial breathing mode of a 320 nm thick optomechanical disk (blue region) and of the fundamental mode of a quasi-spherical biological particle adsorbed on a rigid support (red region), as a function of the disk and bioparticle radii, respectively. **B.** Effect of bacterium adsorption on the radial breathing mode of an optomechanical disk (2.5 μm in radius and 320 nm in thickness). The inset shows a scanning electron microscopy image of the optomechanical disk with an attached Staphylococcus epidermidis cell.

TiO_2-EPE/CTA nanocomposites: solvent casting vs solvent vapour annealing

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Materials based on biodegradable polymers and modified with inorganic nanoparticles are indispensable to reduce the problems generated by plastic waste [1]. However, they are not as competitive as the conventional materials, and therefore employment of different preparation methods are necessary to improve their properties [2].

In this work [3], cellulose triacetate based nanocomposites modified with sol-gel synthesised TiO_2 nanoparticles and EPE triblock copolymer have been prepared by two different methods. In the case of solvent casting (SC) pathway, solutions were cast in petri dishes and kept at ambient conditions until solvent evaporation. On the other hand, in the solvent vapour annealing (SVA) method, nanocomposites were dried in an oven under an acetone vapour atmosphere.

Nanocomposites prepared by SVA presented smoother surfaces than SC nanocomposites, and in consequence, higher gloss values. Moreover, as observed in Figure 1a, they displayed a great surface finish without visible defects and high transparency at 650 nm even at high sol-gel content. As for AFM phase images, they showed that the preparation methods affected the self-assembly ability of the EPE triblock copolymer, and therefore, the morphology of the nanocomposites. In the case of $10TiO_2$-EPE/CTA, SC sample presented a heterogeneous system, whereas SVA films a homogeneous one (Figure 1b). This is reflected in the mechanical properties, since SVA nanocomposites presented higher Young's modulus and tensile strength than SC ones. Finally, UV-shielding properties were not affected by the preparation method.

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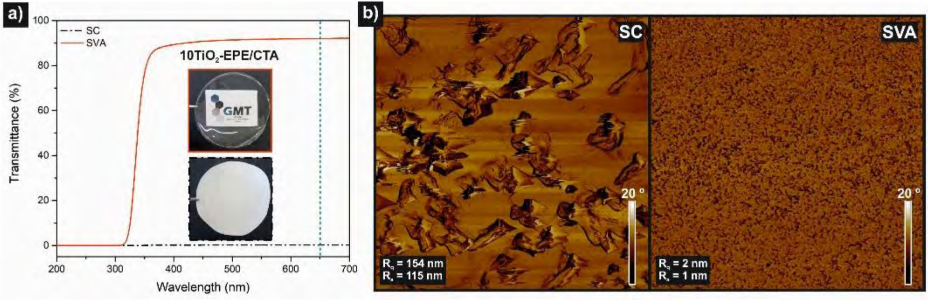

Figure 1: a) UV-vis spectra and digital images and b) phase images (5 µm X 5 µm) of $10TiO_2$-EPE/CTA prepared by SC and SVA.

Incorporation of magnetite nanoparticles in chitosan-based scaffolds for magnetic hyperthermia therapy and bone regeneration.

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There is a high demand to develop new strategies to treat malignant bone tumors and, simultaneously, to regenerate bones defects produced by the tumor resection. Multifunctional bioactive 3-D scaffolds can be a potential approach to fulfill this urgent need. In this work, it is proposed to develop magnetic chitosan-based scaffolds, through freeze-drying, with potential to simultaneously promote bone regeneration and kill residual cancer cells by thermal hyperthermia. Chitosan was selected as main matrix due to its properties suitable for bone tissue engineering, such as biocompatibility, antibacterial, and osteogenic behaviour. Although, it possesses poor mechanical properties, showing low elastic moduli [1]. As Fe_3O_4 NP have been highly explored in biomedical fiel as heat mediators in magnetic hyperthermia therapy, pristine Fe_3O_4 NP produced by co-precipitation could be incorporated in chitosan-based scaffolds to increase their mechanical strength. Therefore, different chitosan concentrations were assessed (1, 1.5, 2 and 2.5% w/v) and the effect of Fe_3O_4 NP incorporation on scaffolds properties were evaluated.

The results show that scaffolds porosity decreases as chitosan concentration increases, although a porosity around ~95% and ~83% were achieved for chitosan at 2 and 2.5 % w/v respectively. On the other side, scaffolds with higher Young Modulus and enhanced toughness were attained for 2.5% w/v since scaffolds with lower porosity exbibits higher mechanical response, improving the scaffold integrity. Synthetized spherical Fe_3O_4 NP with sizes around 9 nm, and with a Specific Loss Power of 98 W/g were then incorporated (10 and 20 % w/w) in 2.5 and 3% w/v chitosan matrix producing magnetic scaffolds. A significant reduction of porosity was only observed for chitosan at 3% w/v with 20% w/w NP (~65.5%). Although, mechanical properties were highly enhanced with an increase from 0.68 to 2 MPa for Young Modulus and from 16.5 to 41.7 MPa for toughness, comparing to pristine chitosan scaffolds. Furthermore, this incorporation did not significantly affect the elongation properties (~23.1%). In general, the results confirm the ability to produce highly porous scaffolds with freeze drying technique, even for higher chitosan concentrations, and the incorporation of Fe_3O_4 NP specially at 20% w/w improves chitosan scaffolds mechanical properties without compromising the porosity. Therefore, these magnetic scaffolds, could have a great potential to address simultaneously the regeneration of bone defect and eradicate residual cancer cells by thermal hyperthermia.

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Kondo lattice development in a TaS_2 van der Waals heterostructure

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Kondo screening occurs when a magnetic impurity is embedded in a metal, below a given temperature, known as the Kondo temperature, a singlet state forms between the spin of the impurity and the spins of the conduction electrons [1]. When the distance between the magnetic impurities is small enough the physics of the system is expected to be modified [2]. The first experimental evidence was obtained in the 1970s in systems containing rare earths [3]. By means of scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperatures we explore a van der Waals heterostructure consisting in a single layer of 1T-TaS_2 on a 2H-TaS_2 crystal. The 1T-TaS_2 layer presents a $\left(\sqrt{13}\times\sqrt{13}\right)R13.9°$ charge density wave (CDW) with a localized electron at the center of every unit cell of the CDW. For temperatures below 28K the spatially resolved STS shows the presence of a Kondo resonance in the Mott-Hubbard gap. For temperatures below 11K the system develops a quantum coherent state called Kondo lattice.

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Figure

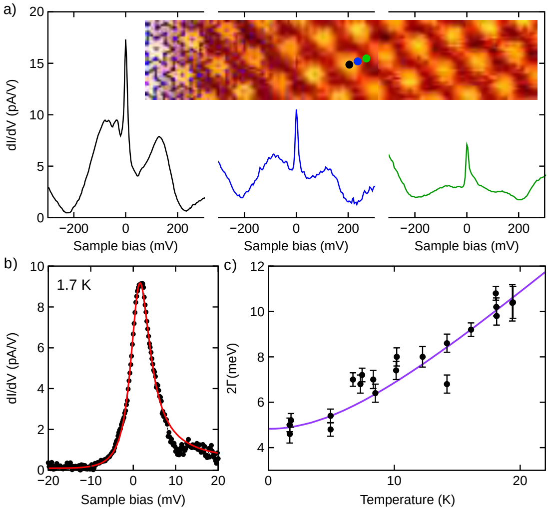

Figure 1: a) Single point STS taken on different locations along the CDW unit cell showing the modulation of the intensity of the zero bias Kondo peak. The Kondo resonance is more intense at the centre of the CDW unit cell (black spectrum) and decays very fast away from the centre (blue and green spectra). STS parameters: 500 mV, 500 pA, Vmod=5 mV. The inset shows the area of the sample where the spectra were measured, with the STS locations colored accordingly. Image parameters: 500 mV, 90 pA, 20 nm x 4 nm. b) Individual spectrum belonging to the temperature series of the panel c), in this case the spectrum is taken at T=1.7 K and fitted with a Fano function taking into account the broadening produced by temperature and the lock-in modulation. c) Plot showing the dependence with temperature of the intrinsic full width at half maximum (FWHM) of the Kondo resonance, and corresponding fit to the expected behaviour according to the Fermi liquid theory, giving a Kondo temperature of T_K=27 K.

Permeation and Recombination of Hydrogen Chemisorbed on Graphene: Insights from Computations

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Recent discoveries that graphene permeates protons[1] and hydrogen atoms[2] have opened up prospects of new applications in hydrogen technologies, energy storage and conversion, isotope separation, etc. In addition, a great interest has risen for uncovering the microscopic mechanisms underlying such observations. In the presentation, we will address two processes involved in hydrogenated graphene, namely, the permeation or flipping of chemisorbed hydrogen atoms through a graphene layer and the recombination of these atoms (desorption and formation of hydrogen molecules, a reaction that can occur after permeation). With the aim to provide some insight into these processes, we have carried out density functional theory computations using large molecular prototypes of graphene. Firstly, we will discuss a new mechanism for the flipping of chemisorbed hydrogen atoms[3] or protons[4] (see Fig. 1), for which the estimated activation energies are of the order of the experimental findings[1,2]. Secondly, we will report reaction paths and rate coefficients for the recombination of hydrogen and deuterium and analyze the large isotopic substitution effects[5] observed in thermal desorption measurements[6,7]. Finally, some findings about the role of Stone-Wales defects on the studied processes will be outlined.

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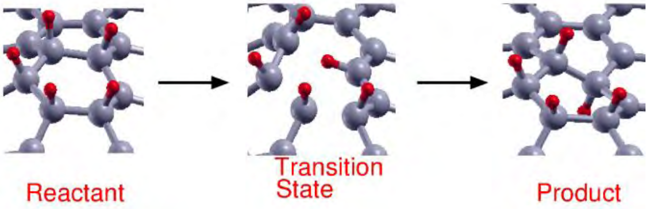

Figure 1: Geometries of the reactant, transition and product states for a hydrogen atom flipping through a highly hydrogenated carbon ring. The activation energy is about 1.5 eV.

Exploiting intrinsic defectiveness in MoS_2-based field-effect transistors for sensing applications: from polycyclic aromatic hydrocarbons to heavy metal ions

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The increasing population and industrial development are responsible for the environmental pollution characterized by a severe contamination of air, water and soil. Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous environmental pollutants which results from the incomplete combustion of organic materials (e.g., coal, oil, petrol, and wood). PAHs' intrinsic properties such as thermostability have made them highly persistent in the environment. Their various health effects have caused the increased concern of the scientific comunity and governmental organizations.

Low-dimensional materials are ideal scaffolds to be used as active components in chemical sensing because they combine a high surface-to-volume ratio with physical and chemical properties that are highy susceptible to environmental changes. The non-covalent recognition events occurring between the low-dimensional nanostructure and the analyte of choice when interfaced, can be used as transduction mechanisms, yielding extraordinary performance in chemical sensing. Among low-dimensional materials, 2D transition metal dichalcogenides (TMDCs) are ideal materials to be integrated in sensors with an electrical readout. By pursuing this strategy, MoS_2-based field-effect transistors (FETs) have been recently proved to be an excellent candidate for heavy metal ion sensing [1].

In this work, we present premilinary results on PAH MoS_2-based sensors, relying on the high affinity between those molecules and intrinsic point defects in TMDCs. X-ray photoelectron spectroscopy (XPS) and low-temperature photoluminescence (PL) showed a significant reduction of the defectiveness of MoS_2 when exposed to different PAHs solutions. Transfer characteristics in the MoS_2 FETs provided unambiguous confirmation that naphthalene acts as a p-dopant for MoS_2. Interestingly, we observed a strict correlation of this doping with low-temperature PL and Raman measurements. The neutral exciton in MoS_2 became more prominent after exposure to PAH solutions. PL signal increased after naphthalene exposure, indicating a p-type doping of the MoS_2 [2]. Along the same line, shifts in the MoS_2 A_{1g} Raman peak were observed after exposure to the solutions, in good agreement with the observed p-doping in the transfer characteristics.

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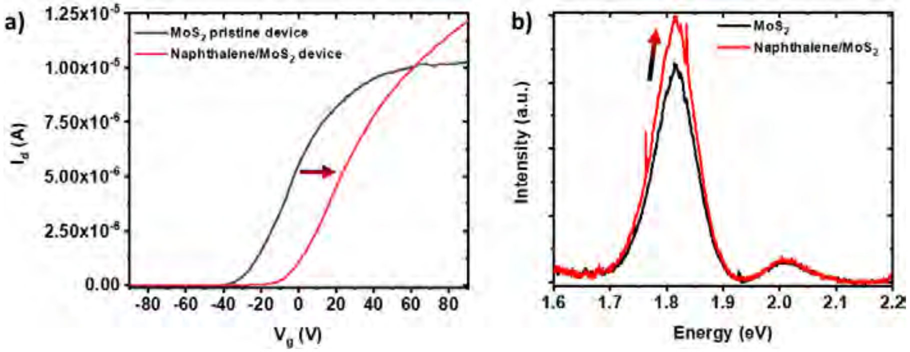

Figure 1: **a)** Transfer characteristic of both pristine (in black) and naphthalene exposed (in red) devices. Threshold voltage shifted towards positive values indicating a p-type doping. **b)** PL characterization of the pristine and functionalized MoS_2 in black and red, respectively. The increase observed in the PL after naphthalene exposure indicates a p-type doping, in good agreement with the electrical characterization.

Effect of intrinsic defects on the thermal conductivity of PbTe

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Despite PbTe being the archetypal thermoelectric material, still today some of the most exciting advances in the efficiency of this and related materials are being achieved by tuning their properties at the nanoscale. Its inherently low lattice thermal conductivity can be lowered to its fundamental limit by designing a structure capable of scattering phonons over a wide range of length scales. Intrinsic defects, such as vacancies or grain boundaries, can and do play the role of these scattering sites. Here we assess the effect of these defects by means of molecular dynamics simulations. For this we purposely parametrized a Buckingham potential that provides an excellent description of the thermal conductivity of this material over a wide temperature range [1] (see Figure 1). Our results show that intrinsic point defects and grain boundaries can reduce the lattice conductivity of PbTe down to a quarter of its bulk value (see Figure 2). By studying the size dependence, we also show that typical defect concentrations and grain sizes realized in experiments normally correspond to the bulk lattice conductivity of pristine PbTe. We then address the issue of the survival of nanostructuring against thermal coarsening using a phase field model [2].

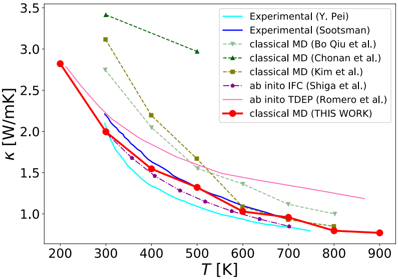

Figure 1: Thermal conductivity of bulk PbTe

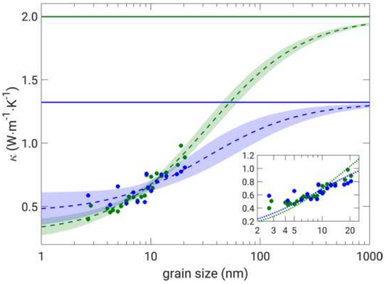

Figure 2: Thermal conductivity of polycrystalline PbTe

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Fabrication of 2D Oxide Nanosheets Structured Ultrathin Capacitors

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The two-dimensional (2D) oxide nanosheets with a wide bandgap have high dielectric properties, and they are single crystals delaminated by chemical exfoliation of bulk layered materials [1]. These crystallites have an approximate thickness of 1 nm and a lateral size of up to 10 µm. Since they can be self-assembled as building blocks, they are promising candidates for applications of next-generation energy storage devices, which need well-organised low-dimensional nanoarchitectures. Studies on Dion-Jacobson type $Ca_2Na_{x-3}Nb_xO_{3x+1}$ nanosheets revealed that an increase in x number will result in an increase in dielectric characteristics according to polar phonon frequency softening [2]. When the perovskite Dion-Jacobson material is synthesised and exfoliated at the maximum x value, new forms of nanosheets with high dielectric properties can be produced. In this study, we have exfoliated Dion-Jacobson-type perovskite layered material of $KCa_2NaNb_4O_{13}$ to obtain the single $Ca_2NaNb_4O_{13}$ nanosheets. The nanosheets were then deposited on ITO flexible substrates grown on PET substrates using the Langmuir-Blodgett technique. The nanosheets structured nanofilms were fabricated by repeating the procedure. Each layer of nanofilms was analysed by the UV-Vis spectrophotometer to confirm the nanofilm growth. The LB nanofilms were patterned by e-beam lithography technique and coated with ITO to develop ultra-thin, flexible, and transparent capacitors. The development of these capacitors will provide new solutions to the miniaturisation problems of silicon-based technologies for flexible display devices.

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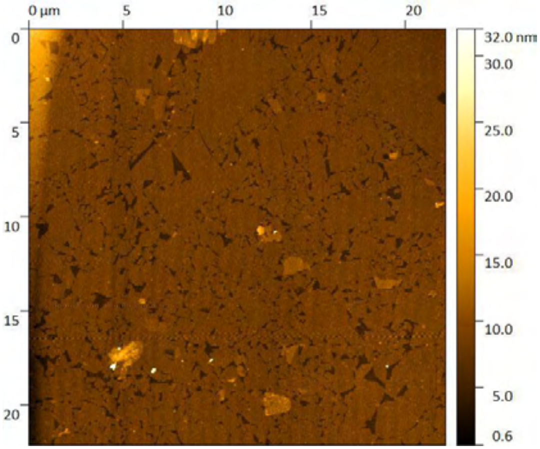

Figure 1. AFM image of LB deposited single $Ca_2NaNb_4O_{13}$ nanosheet monolayer on the silicon substrate

Stimuli responsive Bacterial Cellulose composites

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Raw materials of natural origin and in particular, biopolymers like cellulose play an essential role as eco-friendly materials. Cellulose (C) and nanocellulose (NC)-based materials have emerged as exciting candidates to industries, governments and consumers as green, sustainable and natural materials for the fabrication of advanced complex composites.

Nanoparticles (NPs) can be tuned chemically and structurally to obtain NPs with interesting properties. Combining materials of raw origin, like cellulose, with nanoparticles opens new avenues in developing novel materials that harness nanotechnology and nature.

In this context, we will present our latest development on novel stimuli-responsive materials for various applications based on bacterial cellulose (BC). We explored the modification of BC at the biosynthesis steps during the bacterial cellulose production or ex-situ after the synthesis. We created multifunctional bacterial cellulose laminate materials and spherical BC structures with the confinement of several types of nanoparticles. The possibility to control the content of materials and the structure of the BC expands the palette of interesting biohybrids.

Figures

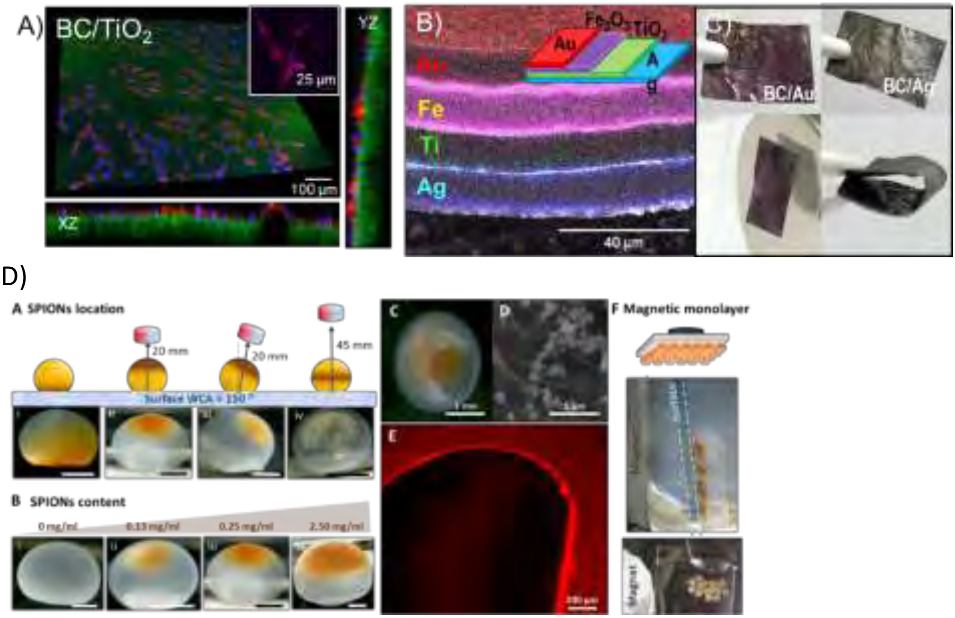

Figure 2: BC Composites of: A) Titania nanoparticles where we cultured fibroblast cells, B) Multilaminate BC composites C) Flexible BC nanocomposites. D) BC spheres composite with SPIONs to afford magnetic responsible biomaterials.

Impact of hierarchical Quatsome-RGD nanoarchitectonic surfaces on integrin-mediated cell adhesion

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The RGD peptide has been widely used in cell adhesion studies due to being one of the main integrin ligands.[1] While RGD has been immobilized with different ligand to ligand spacing in a homogeneous approach,[2] its quantitative effect on cell adhesion when locally clustered on nanocarriers has not been assessed. Quatsomes are non-liposomal nanovesicles proposed as a versatile nanocarrier platform for the nanoarchitectonic immobilization of the RGD peptide on surfaces. Quatsomes functionalized with RGD peptide and a SH group were produced using a technology based on supercritical CO_2.[3,4] Those Quatsomes were anchored on gold surfaces through the gold-thiol interaction, forming SAM structures and used to perform cell adhesion experiments on an osteosarcoma cell line. Substrates were additionally characterized through AFM to assess Quatsome integrity[5] and through EIS to assess the presence and accessibility of the RGD peptides. The immobilization of Quatsomes on surfaces was successful and allowed to present RGD peptides incorporated in its fluid membrane with an enhanced format in comparison with traditionally used homogeneous RGD-functionalized surfaces regarding cell adhesion.[6]

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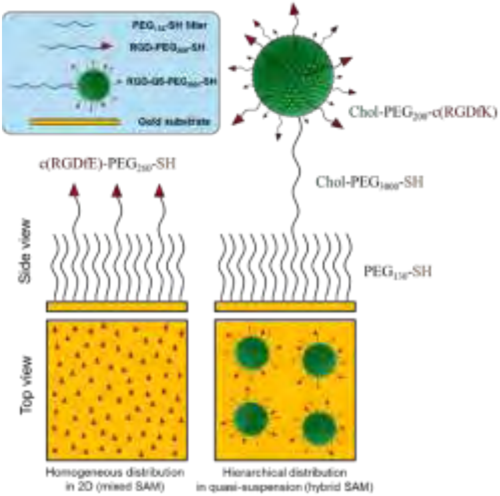
Figure 1: Schematic representation of the produced substrates, featuring either a homogeneous distribution of RGD or locally clustered RGD through Nanocarriers.



Hybrid nanomechanical-microfluidic devices for stiffness and compressibility characterization of in-flow cells

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The developement of versatile tools for measuring multiple physical properties of single micro and nanoparticles is a matter interest in a wide range of fields as material science or solid-state physics. But, biology is perhaps the field demanding the most this kind of tools in the nanoscale. Mechanical properties as mass density or Young's modulus have been demonstrated to be useful parameters not only for discerning among different biological particles, but also because they have a fundamental biological significance [1]. Suspended microchannel resonators (SMR, Fig. 1a) [2] are the result of the convergence of two promising techniques in this scope: microfluidics and nanomechanics. SMR devices have been demonstrated to be really usefull to measure some mechanical properties as mass or density [3]; however, the hydrodynamic forces, widely used in microfluidics, remains unexploited in these devices [4], leading to missing information of high physical and biological relevance.

In this work, we have theoretically studied the hydrodynamic lateral force actuating on a flowing particle crossing a SMR (Fig. 1a) and how this force is transmited to this resonator (hydrodynamic load), changing its resonance frequency. After that, we have elucidated how the SMR devices must be designed so as to compliment the mass measurements with these hydrodynamic forces (Fig. 1b), which have never been measured yet. Moreover, we demonstrate that the measurement of this hydrodynamic load can be used in the case of soft particles (e.g., biological cells, Fig. 1c) to measure mechanical properties as stiffness (Fig. 1c) or compressibility. These results open the door to a new generation of SMR devices capable of performing a simultaneous multiplexed individual cell analysis combining mass and optical [5] characterization with these stiffness measurements.

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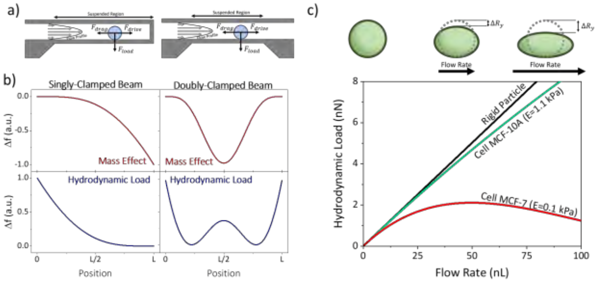

Figure 1: a) Schematic of a singly-clamped (right) and doubly-clamped (left) suspended microchannel resonator and the hydrodynamic forces actuating on a particle crossing it. b) The change in the resonance frequency caused by the passing particles can be divided into two effects: mass effect (red lines, up) and hydrodynamic load effect (blue lines, down). c) Schematic of the effect of the hydrodynamic force on a soft particle shape (up) and hydrodynamic load as a function of flow rate for rigid (black line) and for different cell types (green and red lines).

Laser Induced Forward Transfer (LIFT) printing of conductive and dielectric materials

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Laser-Induced Forward Transfer (LIFT) is a versatile technique, allowing the transfer of a wide range of materials, with no contact, and high accuracy. LIFT allows the use of inks, pastes, and even solid films, as the donor material [1]. It is a promising printing and metallization method for the PV industry. Also, the capability of print both metallic and insulating materials allows the deposition of different circuit elements as capacitors, resistors, or inductors [2].
Here we show a complete study on the deposition by LIFT of different materials (silver paste, cooper ink , graphene ink and ceramic oxide) (see figure 1). Finally, the metallization of PV solar cells by LIFT using a high-viscosity silver paste is presented [3] (see figure 2).

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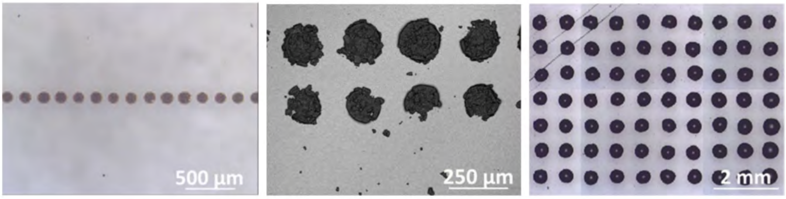

Figure 1: Confocal microscope images of voxels transferred by LIFT of a graphene ink (left), a ceramic oxide (centre) and a copper ink (right).

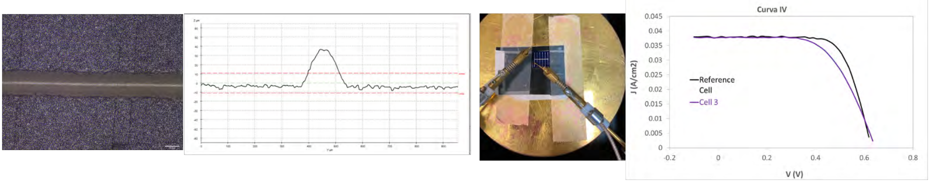

Figure 2: Silver paste line printed by LIFT (confocal image and section profile). Current density-voltage curves of the cells (measured using a solar simulator and four tips).

Engineering bandgap opening in Dirac cone on Graphene/Te heterostructure

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Graphene, in its pristine state, is a semiconductor with a zero band gap and massless Dirac fermions carriers, which conducts electrons like a metal. Nevertheless, the absence of bandgap makes impossible to control the material's electrons, something is essential to perform on-off switching operations in transistors. Therefore, it is necessary to generate a finite gap in the energy dispersion at the Dirac point. An intense research has been developed to engineer band gaps while preserving the exceptional properties of graphene and different strategies have been proposed, among them, quantum confinement of 1D nanoribbons[1] or the introduction of a superperiodic potential in graphene[2]. Besides, in the context of developing new 2D materials and Van der Waals heterostructures, with new exciting emerging properties, as 2D transition metal chalcogenides monolayers, it is fundamental to know any possible interaction between chacogenide atoms and graphene supporting substrates. In this work, we report on a combined Scanning Tunneling Microscopy (STM), Low Energy Electron Diffraction (LEED) and Angle Resolved Photoemission Spectroscopy (ARPES) study on a new superstructure when Te is evaporated on graphene over Ir(111). This new superstructure leads to the electronic doping of the Dirac cone, while the linear dispersion of massless Dirac fermions is preserved. Very interestingly, our ARPES measurements evidence a large band gap (~400 meV) at the Dirac point of graphene Dirac cones, below but close to the Fermi level, as shown in figure 1.

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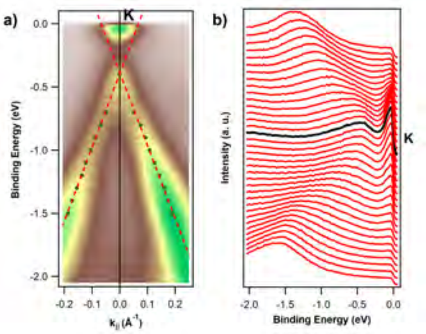
Figures

Figure 1: a) ARPES spectrum at K point of the Gr/Te/Ir(111) heterostructure. **b)** Energy Distribution Curves evidence the gap opening at the Dirac point.



Smart bioevaluation of chemicals and biopolymers using *C. elegans*.

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Introduction

Caenorhabditis elegans (*C. elegans*) is a 1-mm free-living soil nematode with easy experimental manipulation, short life cycle, transparency, and highly conserved genome, which makes it a powerful and informative in vivo model[1]. Here we performed the initial evaluation of the potential use of bacterial nanocellulose fibers[2] (BNCf) as a dietary fiber and the biointeraction of inorganic chemicals[3] designed for different biomedical applications.

Methodology

Regarding BNCf, we studied its toxicity after 24h of exposure and its effects in development, by measuring the final worm's size; genetic expression profile, by RNAseq; and lipid levels by Oil-red-O or bodipy staining. The chemical's toxicity profile was analyzed after 24h of exposure at L4 *C. elegans* stage, obtaining the LD50 by counting the percentage of alive worms. Worms' eggs were exposed 24h and molecules inside them were characterized by different physico-chemical techniques.

Results

BNCf was not reducing the survival rate of worms but BNCf-treated worms wereslightly shorter than controls and had a reduction of lipid levels. Moreover, a significant difference in the genetic expression profile was observed, being the immunological genes activated and mitochondrial genes downregulated. In the case of chemicals, the LD50 was lower than the IC50 obtained in in vitro experiments, and compounds were located in embryos through different characterization techniques.

Conclusion

In both cases, the importance of testing novel compounds in simple models has been proved before going one step further. For BNCf, the *C. elegans* model replicated some of the already observed effects in complex animals, such as the decrease of lipid levels but it also revealed new insights in BNCf's biointeraction such as the upregulation of the immune response genes. In the chemicals' bioevaluation, a different effect in the entire organism in comparison with in vitro studies was observed.

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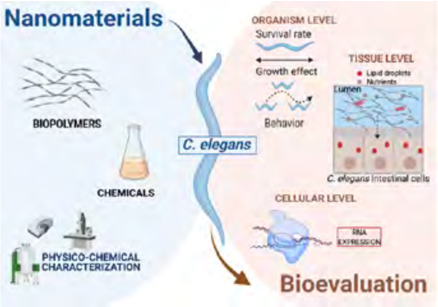

Figure 1.-Graphical abstract of the project.

Linking the macroscopic properties of nanofluids with the interfaces configuration

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Interfaces have a huge influence on the properties of nanostructured materials, and controlling the configuration of the interfaces opens the way for the development of highly functional materials with optimized properties that cannot be achieved at the bulk scale. Nanofluids, colloidal suspensions of nanomaterials in a base fluid, are a good example of this observation. It has recently been proven, through DFT/MD simulations and experimental data, that the chemical interactions between the species of the base fluid and the dispersed nanomaterial affects the thermal conductivity and the specific heat of these nanofluids [1-3], which is of interest for advanced applications of heat transfer and storage. However, choosing the right nanofluid for a particular application is a complex process that requires rationalization.

Thus, in this work, we present the rationalization of the thermal properties, specific heat and thermal conductivity, of the metal-containing nanofluids through both experimental and theoretical perspectives. Pd and Au nanoplates were synthesized (see Figure 1) and nanofluids were prepared using a synthetic oil (the eutectic mixture of biphenyl and diphenyl oxide as the base fluid. These nanolufids were characterized in their properties of interest, colloidal stability, thermal and rheological properties. The chemical configuration of the interfaces was studied through DFT/MD simulations. Thanks to the dual perspective, a correlation between the interactions on the interface and the properties measured was performed. This correlation can allow to predict the nature of the components of the nanofluids for a specific application.

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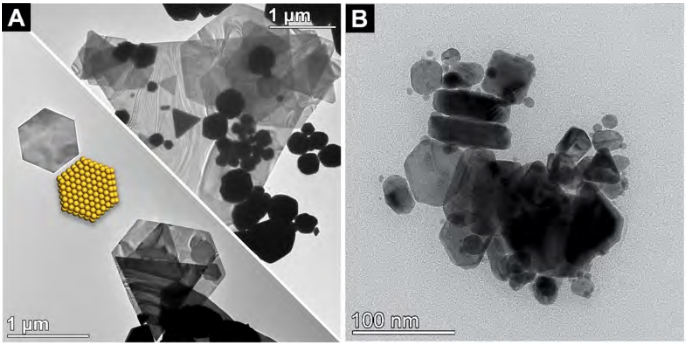

Figure 1: TEM images of gold (A) and Pd (B) nanoplates.

Hexagonal MnBi islands with tunable magnetic anisotropy

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Permanent micro- and nano- magnets find application in devices such as biological probing and MEMS [1]. However, their fabrication typically includes complex processing (e.g. lithography). MnBi is an intermetallic ferromagnetic alloy with good permanent magnet properties such as a high magnetocrystalline anisotropy of 1.6 MJ/m^3 at room temperature and a relatively high $(BH)_{max}$ of 20 MGOe. On top of that, MnBi shows a high Curie temperature of 711 K and an unusual positive temperature coefficient of the coercivity [2-4], which makes it an attractive rare earth-free alternative for high temperature applications.

In this study, a one-step route has allowed for the fabrication of highly crystalline hexagonal MnBi islands (thickness varying from 200 nm to 2.1 µm and lateral dimension of 30 µm), by RF-sputtering of a composite target onto glass substrates at different deposition temperatures (T_D) [4]. A strong impact of T_D on the magnetic properties has been proven. Specifically, magnetic anisotropy could be tuned from out-of-plane ($T_D < 375$ K) to in-plane ($T_D = 475$ K), with no need of an external magnetic field during deposition.

High values of coercivity have been obtained: 13.1 kOe at 400 K along the out-of-plane direction ($T_D = 375$ K) and 14.1 kOe at 400 K along the in-plane direction ($T_D = 475$ K). MFM study has allowed observing a strong perpendicular anisotropy in these islands, which show a hexagonal crater-like shape (Fig. 1). The periodicity of the stripe domains obeys the D = 1.18 * sqrt (T) law in good agreement with theoretical predictions. The dependency of D *vs* T in MnBi thin films reported in literature over the years has been validated through the MFM study of the crater-like shape MnBi islands [4]. Moreover, this study has allowed us to extend the dependency of D *vs* T for MnBi in a thickness range well beyond previously published results, thus advancing in the comprehension of the MnBi system.

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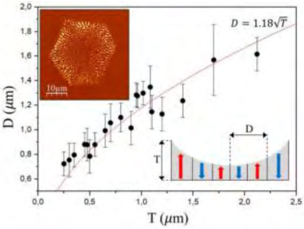

Figure 1: Dependence of domain width (D/2) on the thickness (T) of the islands from MFM images (inset). The D = 1.18 * sqrt (T) law is obtained by fitting the data points (red line).

Acknoledgements

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Thermometry with optical cavities made of luminescent Ga_2O_3:Cr nanowires

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The ultra-wide bandgap semiconductor gallium oxide is currently attracting great interest, mainly for high power electronics [1]. Photonics applications are being parallelly explored, paying special attention to solar-blind UV photodetector applications and tuneable emitters from the near-UV to the IR [1].

In this work, further applications of β-Ga_2O_3 in the field of nanophotonics are explored by designing, optimizing, characterizing and applying optical microcavities created within nanowires [2]. These cavities are based on pairs of distributed Bragg reflectors (DBR) patterned by focused ion beam (FIB) in the nanowires, which results in widely tuneable Fabry-Perot (FP) optical resonances. A complete analysis of their photonic behaviour has been carried out both experimentally and with analytical models, as well as finite-difference time-domain (FDTD) simulations. These approaches are in good agreement with each other and allow to predict and optimize the design and performance of the cavities.

We have developed a novel design of thermometer based on β-Ga_2O_3:Cr microcavities [3]. Thermal shifts of two different PL features are monitored, namely the characteristic R-lines of Cr^{3+} ions and the FP resonances created within the cavity. Each of the mechanisms is optimum for a different temperature range, allowing to sense at least from 150 K up to 550 K. Precision is around 1 K and the full width at half maximum of the FP peaks is nearly unchanged in the whole temperature range. These temperature sensors present a wide dynamic range, high spatial resolution, very high thermal and chemical stability and can be used in harsh environments, ideal for high electronic/optical power devices, among other applications.

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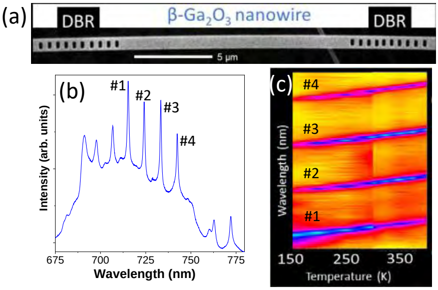

Figure 1: (a) Optical cavity created in a β-Ga_2O_3:Cr nanowire, (b) room temperature local micro-photoluminescence spectrum, (c) FP peak positions dependence on temperature.

Novel and Sustainable Manufacturing of Nanocrystalline Ferrite Permanent Magnets through Recycling and Additive Manufacturing

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Permanent magnets (PMs) based on ferrites are the most used due to their availability and low cost, being an alternative to PMs based on critical rare-earths in new applications such as electromobility [1]. This study will show the possibility of fabricating objects by 3D-printing using nanostructured Sr-ferrite powder obtained through recycling of the residue generated from the fabrication of commercial ferrite magnets. Tuning the morphology and structure of the residue by post-processing made possible to obtain Sr-ferrite nanocrystalline powder with PM properties superior, not only to the residue precursor, but to those of the brand-new commercial powder (3.5 fold increase in coercivity and a 25% increase in remanence) [2].

The recycled Sr-ferrite was used as starting material for the synthesis of composites by solution casting [3], and extruding filaments (Fig. 1a) for advanced manufacturing of magnets (with a particle content up to 65 wt%) by Fused Filament Fabrication technology. Scanning Electron Microscopy (SEM) analysis showed a homogeneous distribution of the particles in the polymer matrix. The magnetic characterization of the composites, filaments and printed objects by Vibrating Sample Magnetometer (VSM) showed that the magnetization scales to the content of ferrite particles (Fig. 1b) and that there is no deterioration of the PM properties of the starting particles along the processing (Fig. 1c) [4]. This work has shown an efficient route for developing new and alternative PMs by the combination of recycling and 3D-printing.

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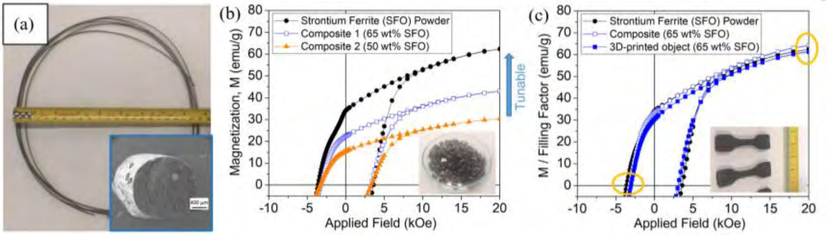

Figure 1: (a) Extruded filament (65 wt% of SFO) and SEM image showing its circular cross section; (b) first and second quadrants of the hysteresis loops of starting powder and composites (image in inset) with different content of ferrite; and (c) normalized hysteresis loops of the starting powder, composite and 3D-printed object. Inset shows 3D-printed pieces for tensile tests based on ferrite particles.

Acknowledgments

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Quantification of TDP-43 in lymphoblasts from ALS patients and their exovesicles with QD-based multiplexing approach

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Amyotrophic Lateral Sclerosis (ALS) is a lethal neurodegenerative disease characterized a progresive loss of motor neurons, that yields muscle tone waste leading to paralysis. Currently, drug development is hampered due to the heterogeneity of the disease and the lack of knowledge of the mechanism triggering selective motor neuron death. TDP-43 is the main affected protein in ALS. Physiologically, TDP-43 is located at the nucleus, and in ALS, it is found aggregated in the cytoplasm. [1].

Molecular profiling is an innovative powerful technology for unravelling complex molecular pathways that underlie physiological and pathological processes. Quantum dots (QDs) are luminescent nanoparticles with a high potential to become promising tools to detect molecular mechanisms at the subcellular level enabling multiplexing applications.[2]

After studying QD penetration properties in lymphoblasts derived from patients, we determined that the nuclear penetration of antibody-conjugated QDs can be controlled [4] and thus an efficient manner to target ALS pathologic TDP-43 has been developed. This enables an automated rapid analysis of TDP-43 and its relation to other ALS key targets by immunofluorescence and the possibility of quantification by flow cytometry. Here we implement this methodology and study ALS pathology in this model derived from patients and its modulation upon drug treatment, as an approach towards personalized medicine in ALS starting from patient derived models. Finally we use these nanoparticles to phenotype exovesicles in our model of ALS.

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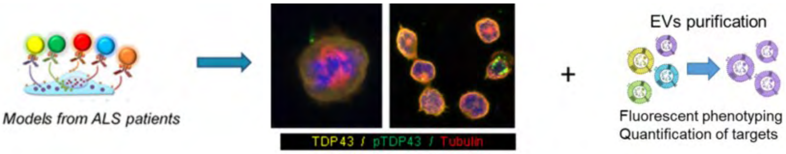

Figure 1: QDs multiplexing in lymphoblast from ALS patients targeting TDP-43 and analysis and phenotype of their exovesicles.

Advanced In Situ Transmission Electron Microscopy: A powerful tool for materials science, catalysis, energy storage & lifescience applications

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We introduce our technology for in situ studies inside transmission electron microscope (TEM), where next to heating and biasing studies, also environmental studies (i.e. in gaseous or liquid environments) are made possible. The systems rely on a Micro Electro-Mechanical System (MEMS)-based device as a smart sample carrier, which contains an integrated set of biasing electrodes or an integrated microheater, to enable in situ electrochemistry, catalytic studies, failure analysis and biomedical studies, among others. As a result, the system provides users with the capability to visualize exciting dynamics in vacuum or liquid/gas environments as a function of different stimuli. In order to provide meaningful results and address historical challenges, our MEMS device controls the flow direction and ensures the gas/liquid will always pass through the region of interest. Thereby, the developed systems offer the opportunity to define the mass transport and control the kinetics of the reaction. Furthermore, the systems allow to control the liquid thickness, enabling resolutions that can go even down to 2.15 Å (for a 100nm liquid thickness). We believe that our developments will play a fundamental role in addressing many of the research questions within battery optimization, fuel cells, (electro)catalysis, as well as for advanced (bio)materials and nanomedicine. Furthermore, it will the unique possibility to visualize biological processes in real time, without the need of vitrifying the biological specimen.

Keywords: Transmission electron microscopy, in situ, MEMS, environmental studies, stimuli

Figures

Optically induced sensing of memristors based in LSMO/BTO/ITO ferroionic tunnel junctions

Isabel Tenreiro,[1] Víctor Rouco,[1] Gabriel Sánchez-Santolino,[1] Fernando Gallego,[2] Carlos Leon,[1] **Alberto Rivera-Calzada**,[1*] Ivan K. Schuller,[3] and Jacobo Santamaria[1]

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The low power sensing of the non-volatile resistive states of memristors is an important challenge for the implementation of energy efficient neuromorphic computing. Ferroionic tunnel junctions are known to have a resistive switching mechanism ruled by the reversible build up of a Schottky barrier, causing the voltage-driven modulation in the resistance of the different memristive states [1]. In this work we take advantage of the Schottky barrier to get an active reading of the memristive states in a $La_{0.7}Sr_{0.3}MnO_3/BaTiO_3$/ITO ferroionic tunnel junction with a 3 nm thick $BaTiO_3$ layer [2,3]. The Schottky barrier formed in the $BaTiO_3$ layer dramatically enhances its optical sensibility and produces a photovoltaic response when illuminated with a UV LED, which open circuit voltage V_{oc} correlates linearly with the resistance of each state, enabling the active sensing of the memristive state.

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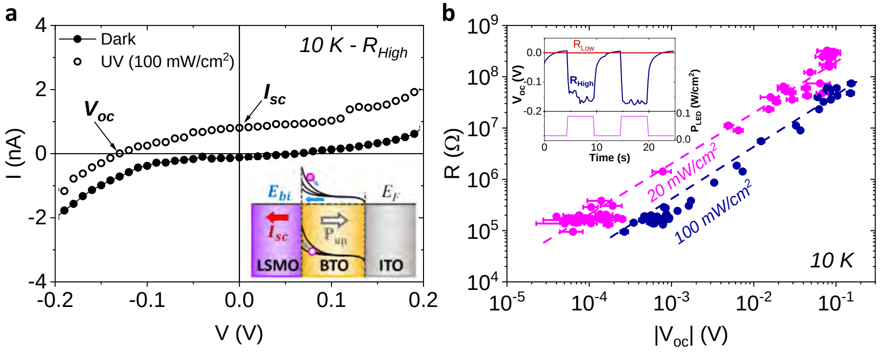

Figure 1: (a) I-V curves in the RHigh in dark and under UV illumination. Inset is a sketch of the band diagram, indicating the variation of the Schottky barrier for different memristive states. (b) Resistance of different memristive states at 10 K as a function of the measured $|V_{oc}|$. Dashed lines are guides for the eye with slope 1 corresponding to a linear correlation. The inset shows the time resolved V_{oc} for R_{High} and R_{Low} memristive states, measured under 5 seconds light pulses.

Piezoelectric flexible materials supported by hierarchically porous graphite for sensor applications

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Piezoelectric materials' capacity to convert mechanical energy into electrical stimulus is nowadays very attractive for sensing and energy harvesting. Piezoelectric composites combine mechanical flexibility and high electromechanical coupling constants, which are desirable in wearable devices; nonetheless, polarisation may be compromised due to the polymer's low dielectric constant and the ceramic phase's discontinuity. While the dielectric discrepancies may be rectified using conductive carbon nanoparticles, the low connection between the piezoelectric phase remains unresolved [1]. Recently developed, highly porous 3D carbon networks are thought to address these concerns [2]. This work will investigate an entirely new concept for designing and fabricating piezoelectric flexible materials using a 3D graphite network loaded with barium titanate and impregnated with a flexible biobased polymer.

Barium titanate particles were synthesised through hydrothermal synthesis at a moderate temperature (200 °C), and the effect of reaction time on the tetragonality of the particles was investigated to optimise this process (conventional and microwave-assisted synthesis). X-ray diffraction and Raman spectroscopy were used to determine the structural phase, while scanning electron microscopy (SEM) was used to evaluate the morphology. The barium titanate particles were impregnated into the graphite network with and without the use of voltage, which is believed to enhance and facilitate the impregnation flux. The final device warranted a chitosan/zein polymer to incorporate the resulting apparatus for flexibility with built-in electrodes for electrical output testing. The graphite network piezoelectric responses, preceding and following impregnation (Figure 1), were tested using Piezoresponse Force Microscopy (PFM) and piezoelectric sensitivity measurements. The structure : property relationship was also evaluated.

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Figures

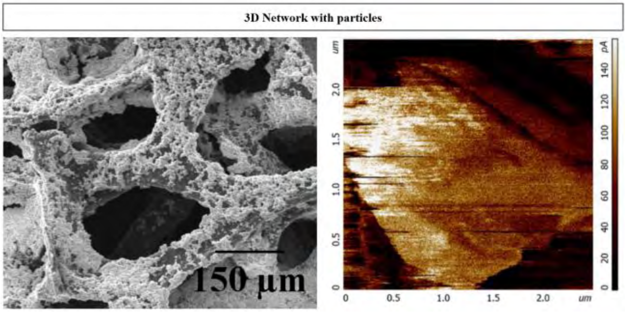

Figure 1: SEM and PFM analysis of the 3D carbon network with particles.

Mechanical disassembly of viral cages probes the interaction of single stranded RNA and the coat proteins

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High resolution cryo-electron microscopy structures of nucleocapsids qualitatively indicate the interaction degree between single-stranded (ss) RNA and coat proteins (CPs) in viruses but lack the direct evaluation of its effects on the virus capsid. Here we study the mechanical uncoating of three variants of the human picobirnavirus(hPBV) virus-like particles (VLPs) which differ in the N-terminal of their CPs: (i) hPBV CP contains the full-length CP sequence; (ii) hPBV Δ45-CP lacks the first 45 N-terminal residues; and (iii) hPBV Ht-CP is the full-length CP with an N-terminal 36-residue tag that includes a 6-His segment. We used Atomic Force Microscopy (AFM) to induce and monitor mechanical disassembly of individual hPBV particles. First, whereas Δ45-CP particles that lack packaged ssRNA exhibited a fast post-breakage indentation, CP and Ht-CP particles that pack ssRNA showed a gradual behavior after being fractured. Second, mechanical fatigue experiments revealed that the increased length of N-terminal (Ht-CP) in 8% makes the virus particles to crumble ~10 times slower than wild type N-terminal CP, indicating an enhanced RNA cargo retention after Ht-CP particles have been crack-opened. Our results indicate that the three differentiated N-terminal topologies of the capsid lumen result in distinct disassembly dynamics as a consequence of their particular interaction with the packaged RNA.

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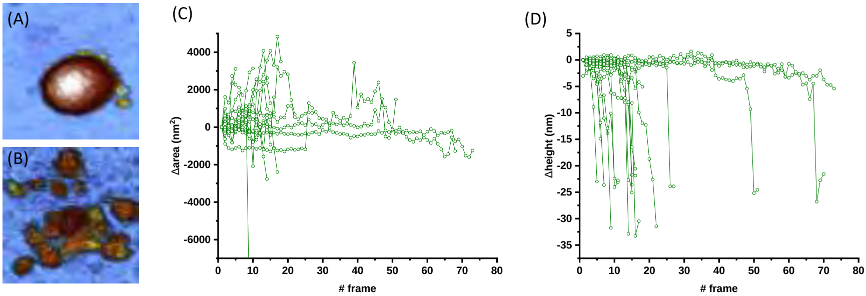

Figure 1: Evolution of an individual CP particle under mechanical fatigue procedure. (A) Frame #0 shows the intact particle, (B) frame #12 is the image of the final collapsed state. (C) Evolution of the particle surrounding covered area with debris for CP VLP. (D) Evolution of the particle height for CP virus particle.

Targeting Myocardial Fibrosis with a Novel Nanotherapeutic System

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A novel anti-fibrotic therapeutic peptide-nanocluster cTPR390-Nluc particle[1,2] is utilized to be incorporated to fluorescent nanocarriers to study its arrival to the heart inside engineered manipulated extracellular vesicles (f-EVs) to treat directly cardiac fibrosis. F-EVs from NIH-3T3 cells were selected to promote addressing them to the heart. Fibroblasts will be the target of the therapeutic system, due to their augmented presence in the pathological situation of myocardial fibrosis.

f-EVs were isolated by differential centrifugation and characterized by flow cytometry, western blot, dynamic light scattering, electron and confocal microscopy. The nanocluster was encapsulated by electroporation and the procedure was verified by flow cytometry. Fluorescence and bioluminescence in vivo imaging was used to visualize the therapeutic system in an animal model of cardiac fibrosis based on Angiotensin-II administration.

At 2 hours after administration, f-EV fluorescence and cTPR-Nluc bioluminescence were co-localized in the heart and lungs. After 6 days after administration, f-EV fluorescence was only visualized in the liver, stomach and intestine.

We conclude that the antifibrotic nanosystem composed by f-EVs and cTPR-Nluc is a fine system to reach the heart of fibrotic mice and a potential theragnostic complex molecule to be translated to clinics.

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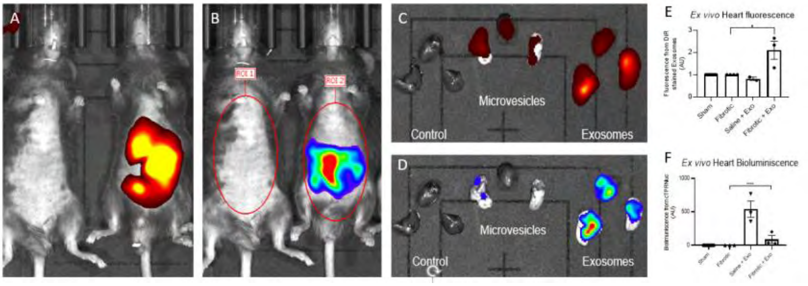

Figure 1: A.: *In vivo* fluorescence detection of f-EVs (exosomes) loaded in cTPR-Nluc after 2 hours of i.p. administration (control left mouse; treated right mouse). B.: *In vivo* bioluminescence detection of cTPR-Nluc loaded in exosomes after 2 hours of i.p. administration (control left mouse; treated right mouse). C.: *Ex vivo* detection of f-EVs fluorescence in the heart (top) and lungs (bottom) after 2 hours of i.p. administration. D.: *Ex vivo* detection of cTPR-Nluc bioluminescence in the heart (top) and lungs (bottom) after 2 hours of i.p. administration. E.: *Ex vivo* quantification of fluorescence detection of f-EVs (exosomes) loaded with cTPR-Nluc after 2 hours of i.p. administration F.: *Ex vivo* quantification of bioluminescence detection of cTPR-Nluc loaded in exosomes after 2 hours of i.p. administration.

Imaging and understanding metal organic frameworks using advanced scanning electron microscopy techniques

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Metal organic frameworks (MOFs) are a structurally tuneable class of hierarchical porous materials with a wide range of host-guest chemistry. Their design acts as a platform for advanced functional materials resulting in properties ranging from charge conductivity, catalytic metal centres, high surface area and organic capacitance. As a result, MOFs have a wide range of applications and can be employed in catalysis, health care, batteries, supercapacitors, and carbon capture[1].

Due to their organic and porous nature, MOFs are incredibly difficult to structurally characterise using typical scanning electron microscopy methods. Beam stability, along with non-conductive nature and porous framework result in a combination of problematic issues for nanoimaging and structural milling.

An example of the degradation MOFs suffer from is electron beam interaction causing surface damage as well as difficulty in imaging of nanoscale structures due to charging artifacts. Alongside this the amorphous nature of adsorbing MOFs results in severe sensitivity to electron beam current resulting in material loss and degradation. The preparation of MOF composite TEM lamellae by FIB milling can prove time consuming and laborious.

Herein we demonstrate a novel technique to imaging, 3D volumetric chemical analysis and TEM lamellae preparation using MOF-74 type analogue for carbon capture and mixed membrane composite CPO-27-Ni in collaboration with the University of St Andrews and the University of Cambridge [2,3]. Using imaging strategies that include high resolution variable pressure microscopy with optimised beam path lengths using NanoVP charge reduction mode, we demonstrate superior imaging at a low vacuum, improving imaging quality and eliminating sample charging and low accelerating voltage to reduce material degradation. Alongside this we employ a cryogenically cooled *in situ* stage to undertake 3D volumetric analysis of a MOF composite membrane in conjunction with energy dispersive x-ray spectroscopy. In doing so we show a new methodology for TEM lamellae preparation, 3D volumetric analysis of MOF composites and best practice imaging using low pressure, low kV scanning electron microscopy.

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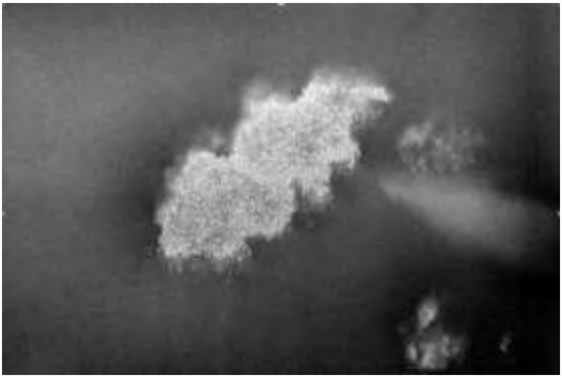
Interactions between CPO-27-Ni and Polyurethane and Their Impact on Nitric Oxide Release Performance. ACS Applied Materials & Interfaces, 12(52).

Figures

Figure 1: cryogenically cooled *in situ* stage to undertake 3D volumetric analysis of a MOF



Influence of Flake Thickness and Environment on Heat Dissipation Capabilities of Suspended $MoSe_2$ Single Crystals

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Transition metal dichalcogenides (TMDs) are layered, two-dimensional (2D) semiconductors which hold promises in future (opto)electronic devices. Importantly, 2D materials can be thinned down to the monolayer, typically with sub-nanometer thickness. Recently, thermal transport properties of TMDs have gained considerable attention because of their anisotropic nature [1]. However, a deep understanding of heat flow in TMDs is missing even though such understanding is crucial to fully exploit them in device applications [2]. In this work [3], we use Raman thermometry to systematically study the effects of flake thickness (0.7–50 nm) and its environment (vacuum, air or N_2) on the thermal transport properties of single-crystalline $MoSe_2$ flakes suspended over large, circular apertures (177 µm^2). Our results suggest that, in vacuum, the in-plane heat flow has a similar thermal conductivity (κ) at 400 K in mono- and few-layer flakes (~20 W/m/K), as in their bulk counterparts (~30 W/m/K). This is due to the appearance of low frequency (~0.1 THz) heat-carrying phonon modes that compensate for the decreasing contribution of interlayer phonon modes (~1 THz) in the thinnest TMDs. Owing to the surface-to-volume ratio increase with decreasing thickness, efficient out-of-plane heat transfer to air or N_2 molecules results in an apparent thermal conductivity (κ_{app}) enhancement of up to one order of magnitude (~200 W/m/K for monolayer flakes) [3]. These findings may provide clear pathways to engineer heat flow in (sub-)nanometer TMDs that are significantly thinner than the smallest state-of-the-art Si structures.

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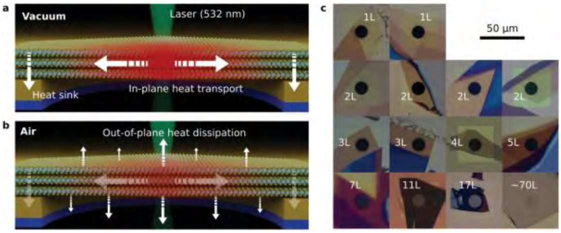

Figure 1: Raman thermometry experiment schematized in **(a)** vacuum and **(b)** air. A laser heats and monitors the temperature of a suspended flake to extract the thermal conductivity. A higher (lower) temperature corresponds to a less (more) efficient heat dissipation. **(c)** Optical images of the suspended few-layer $MoSe_2$ flakes studied in this work.

Functionalization of T-cells with microwave synthesized magnetic nanoparticles for their magnetic retention

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Abstract

Introduction

Adoptive T-cell transfer (ATC) therapy, despite being promising against cancer, has a big drawback: the low proportion of T cells that reach the tumour. To tackle this problem, approaches that localize T lymphocytes in target regions are being tested, such as those based on magnetic nanoparticles (MNPs) [1, 2]. This work evaluates if human and mouse T-cells, functionalized with innovative microwave synthesized MNPs without disrupting their biology, could be retained by an external magnetic field (EMF, magnet).

Methodology

MNPs of different sizes were obtained by microwave-assisted synthesis and coated with aminopropylsilane (APS) and aminodextran. After physicochemical characterization, the biocompatibility between human (Jurkat) or mouse (primary $CD8^+$) T-cells and MNPs were analysed by different experimental approaches: citotoxicity (PrestoBlue assay), iron-association kinetics (ICP-OES), cell localization (confocal microscopy) and the cell surface phenotype (flow cytometry). Finally, magnetic retention of T-cells was studied *in vitro* using a flow chamber system in presence of EMFs.

Results

All microwave synthesized MNPs showed low toxicity and greater iron association to T-cells at 2-4 hours. Also, MNP treatment did not affect the cell surface phenotype of T-cells, and, regarding their localization, confocal microscopy showed that MNPs were present on cell membrane. Among different microwave synthesized MNPs, only APS coated 30 nm particles showed a magnetic retention capacity similar to coprecipitation MNPs of around 10 nm. Together, these data suggest the implications of coating and size in magnetic targeting.

Conclusions

Microwave synthesized MNPs are biocompatible with human and mouse T-cells. Further, when applying an EMF, cell magnetic retention is shown preferentially with a microwave synthesized ~ 30 nm MNP coated with APS (MW1-APS) similarly to coprecipitation ~ 12 nm COP-APS. Although microwave and coprecipitation synthesis methods showed similar results, microwave-assisted synthesis is a more feasible and reproducible procedure and, thus, a more suitable method to be used in clinical practice.

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Structure and magnetism in ultra-thin Fe films on Re (0001)

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The magnetic properties of ultrathin metallic films often deviate strongly from the bulk behavior due to the reduced coordination number of the surface atoms, with results as remarkable as the antiferromagnetic order observed in Fe, a prototypical ferromagnet [1]. Depending on temperature and pressure, iron can present three different equilibrium phases: the α-Fe phase which shows a BCC structure and ferromagnetism at RT, the γ-Fe phase exhibiting an FCC arrangement and can be ferromagnetic under certain conditions, and the ε-Fe phase with an HCP structure. The magnetism of this phase depends strongly on the structure and both ferromagnetic and non-magnetic ordering have been reported in previous works. Theoretical works have reported that ferromagnetism in HCP iron is possible for lattice parameters larger than 2.70 Å and non-magnetic or anti-ferromagnetism is possible for smaller lattice parameters [2], but both phases are almost degenerated in energy.

Here we present a morphological, structural, and magnetic characterization of Fe thin films [1-6 atomic layers (AL)] on Re (0001). The morphology and the growth mode of the films were studied by LEEM and LEED at two different temperatures ranges. Results show that at high temperatures it is possible to obtain a layer-by-layer growth up to the third layer. LEED and LEED-IV fits provided the crystalline structure of the films during the growth. The first Fe layer shows a hexagonal lattice and a hcp stacking sequence following the Re (0001). Second and thicker layers relax their lattice parameter to iron bulk. The magnetic characterization was carried out by both XMCD and XMLD-PEEM measurements. Contrary to recent STM reports [3], no anti-ferromagnetism was found for 1 or 2 AL. On the other hand, XMCD shows ferromagnetism for three or thicker layers.

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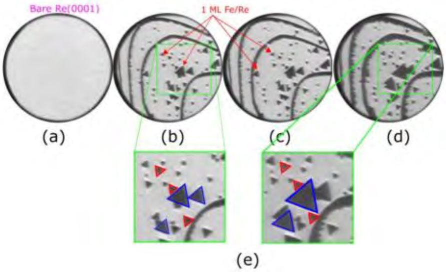

Figure 1: (a)--(d) LEEM images acquired during the nucleation of 1 AL Fe/Re(0001). Fe nucleates on Re as triangular islands with two different orientations in the same terrace. FOV is 10 µm.

Simultaneous optical and mechanical sensing based on nano-optomechanical disks

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A variety of optical and mechanical resonators have been successfully employed in a diversity of sensing applications. Optical resonators stand out for being extraordinary sensitive, while mechanical resonators are highly reliable. In this sense, optomechanical devices are unique platforms, since they simultaneously support high quality optical and mechanical modes. Here we prove that bringing together optical and mechanical resonances in a unique sensing platform, significantly improves the sensor assets, together with its reliability and robustness. In particular, we apply nano-optomechanical disks, which have already shown excellent capabilities when operating in liquids and for biosensing applications [1, 2]. We first apply them for monitoring environmental changes. Notably, the dual sensing approach allows decoupling relative humidity and temperature changes, reaching extraordinary precision, 0.01 % and 100 μK respectivelly. To further prove the capabilities of this novel method, we employ it for detecting individual bacteria (Figure 1). The technique allows to simultaneously access the bacterium optical and mechanical properties, accesing to its mass, rigidity, viscosity, refractive index and absorption coefficient [3].

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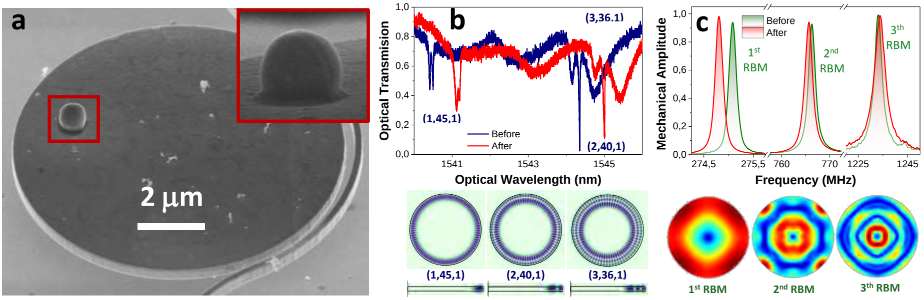

Figure 1. a. Scanning electron microscopy (SEM) image of a nano-optomechanical disks (5 μm in radius, 320 nm in thickness) with an adsorbed *Staphylacoccus Epidermidis* bacterium. The inset shows a zoom of the bacterium. **b.** Optical spectra of the nano-optomechanical disk before (blue) and after (red) the adsorption of the bacterium. Each deep corresponds to a particular whispering gallery mode (WGM) labeled by the interger numbers (p,m,l). The images bellow show the simulated electric field distribution associated to each WGM. **c.** Mechanical spectra of the nano-optomechanical disk before and after the adsorption of the bacterium, showing three resonances corresponding to the first three radial breathing modes (RBM). The images bellow show the simulated displacement field associated to each RBM.

First results on improving the efficacy of magnetic hyperthermia using non-sinusoidal alternating magnetic field waveforms

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Abstract: Recently, efforts have been made to improve the efficacy of particle-mediated magnetic hyperthermia by modifying the waveforms of electromagnetic radiation. Theoretical studies[1,2] propose that trapezoidal waves can improve the thermal power generated with respect to that explained by the classical model for sinusoidal waves[3]. Experimental advances based on new equipment implementing non-sinusoidal waves have also led to some promising results[4,5,6,7]. The first results obtained so far on in vitro samples, on thermal power characterization experiments to study the thermal efficiency of non-sinusoidal stimulation (Figure 1, 2) and on efficiency characterization experiments in cell cultures with cancer cell lines are presented. Although the data obtained are promising, it is also concluded that it is necessary to progress in the understanding of the thermal dissipation phenomenon with non-sinusoidal signals, as well as to improve the prototypes themselves to achieve greater flexibility and power. The most promising avenues for improvement are discussed.

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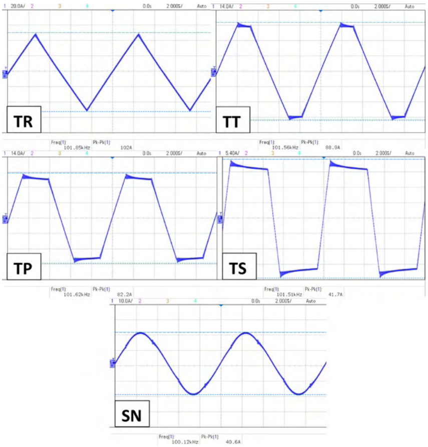

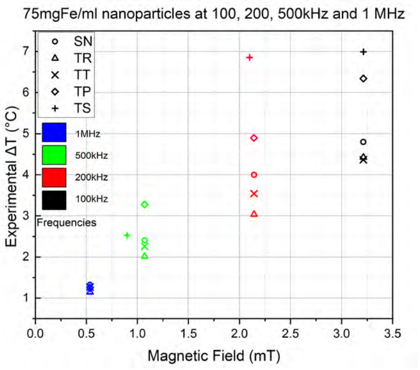

Figure 2: Comparing the 900 second experiment results of all signals at 0.53, 1.07 (except for TS at 0.890), 2.14 and 3.21 mT and 1 MHz, 500, 200 and 100 kHz frequency, respectively.

Tuning the nanoscale architecture in NdFeB ultrathin films with varying buffer layer

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Rare-earth transition metals thin films attract a lot of attention due to their high magnetic anisotropy that makes them excellent candidates for several applications including high density magnetic recording [1-2], microelectromechanical systems and actuators [3] and novel spintronic devices [4]. These next-generation micro-/nano- permanent magnet systems require exploring new synthesis paths that move beyond conventional methods and allow their study with a detailed control over composition, interfaces and microstructure [5]. Our study focuses on the understanding of the mechanisms involved in the formation of the $Nd_2Fe_{14}B$ phase in thin films (5-15 nm) grown by Molecular Beam Epitaxy (MBE) and the possibility of tuning their magnetic response. For this purpose, different buffer layers (Molybdenum and Iron) on MgO (001) have been explored to induce different lattice strains on the NdFeB lattice.

The epitaxial character of the samples has been corroborated by X-Ray Diffraction (XRD) and *in situ* Low Energy Electron Diffraction (LEED) measurements. Magnetic characterization has been carried out by Vibrating Sample Magnetometer (VSM) demonstrating the possibility of inducing a strong magnetic anisotropy in good accordance with the epitaxiallity of the films. A thorough stoichiometric and electronic characterization has been carried out by both X-ray and Ultra-Violet Photoelectron Spectroscopy (XPS and UPS, respectively) also providing values of the work function of the system which, to authors' knowledge, were not previously reported in the literature. Scanning Electron Microscopy (SEM) shows meaningful differences by changing the underlayer: from arrays of highly oriented nanoislands (Fe underlayer, Fig.1c) to low roughness quasi-continuous films (Mo underlayer, Fig. 1d). The understanding and optimization of the nanoscale architecture in these NdFeB thin films is essential when aiming at its integration in novel miniaturized devices (e.g., microdevices for *in vivo* microsurgery applications [6])

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Figures

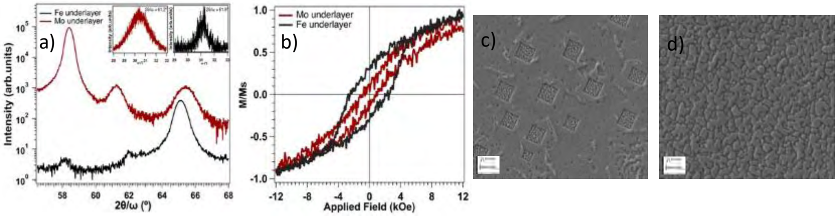

Figure 1: a) XRD pattern of a NdFeB thin film with Fe and Mo underlayer and ω scan of NdFeB (008), b) Out of plane hysteresis loop, c) SEM image of NdFeB with a Fe underlayer and d) SEM image of NdFeB with a Mo underlayer

Acknowledgements

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Electromechanical photophysics of protein fluorophores packed inside individual viral protein cages

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The use of protein virus capsids for packing biomolecules has opened new venues for studying their function in confined environments. They not only mimic the highly crowded conditions in nature, but also allow their exquisite manipulation at the nanoscale for technological applications.

Here, we pack green fluorescent proteins in virus like particles derived from P22 bacteriophage procapsids at high packing fractions and use their emission signal to monitor molecular functionality by Total Internal Reflection Fluorescence Microscopy (TIRFM) while changing the microenvironment of individual capsids with the stylus of an Atomic Force Microscope.

With this simultaneous correlative microscopy at the nanoscale, we could identify two phenomena: a) a mechanical quenching of ~10 %, b) an additional electronic quenching of ~10 % when metallic probes were used. Although fluorescence quenches and recovers after the conductive tip releases the capsid no matter its structural integrity, in the insulator tip's case quenching happens only if the capsid keeps the local organization of the packed protein. Electronic quenching is associated with the coupling of the protein fluorescence emission with the tip surface plasmon resonance while the mechanical quenching is a consequence of the unfolding of aggregated proteins during the mechanical disruption of the capsid. Here we probe the performance of highly packed GFPs whose aggregation facilitates the reversible suppression of their function under mechanical stress, but remains dispensable under electronic stimulus.

Bacterial Nanocellulose-Polypyrrole (BC-Ppy) composites as scaffolds for cardiac resynchronization

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Introduction

Myocardial infarction leads to improper electrical impulse propagation across cardiac cells [1]. Therefore, electrically conducting polymers such as Polypyrrole are promising for cardiac tissue engineering, owing to its easy synthesis, aqueous stability & biocompatibility [2]. Whereas, Cellulose with ECM mimicking fibrous morphology, high flexibility & mechanical strength is ideal as cardiac scaffolds [3]. Here, we designed & evaluated BC-Ppy composites as potential scaffolds for cardiac tissue engineering.

Experimental Methods

BNCs were produced from the bacterial strain Komagataeibacter xylinus (K. xylinus) [4] and BC-Ppy via in-situ oxidative polymerization. The scaffolds were characterized by FT-IR, SEM, TEM, TGA and 4-probe keithly instrument to study their size, structure, morphology and conductive properties. Scaffolds are being tested in-vitro using cardiac fibroblasts and cardiomyocytes.

Results

BNC-Ppy scaffolds were synthesized and found to be ≈ 70 nm BC fiber diameter and that of Ppy NPs ≈ 85 nm. The conductivity of BC-Ppy films were found to be proportional to the concentration of initial monomer added, and was ≈ 10-3 S/cm. In-vitro cell culture experiments with BNC-Ppy scaffolds are at the initial stage studying the viability, cell attachment, morphology etc.

Conclusion

Only a handful studies have shown the efficacy of composites with Ppy as cardiac tissue engineering scaffolds and BNC has not been explored as an effective composite material for this purpose till date. In this work, the intrinsic electrical conductivity, along with excellent biological and mechanical properties of the material is studied for their favorable environment for cardiac cell culture. To the best of our knowledge, this will be a first of its kind study the use of BNC-Ppy as a scaffold for cardiac cells.

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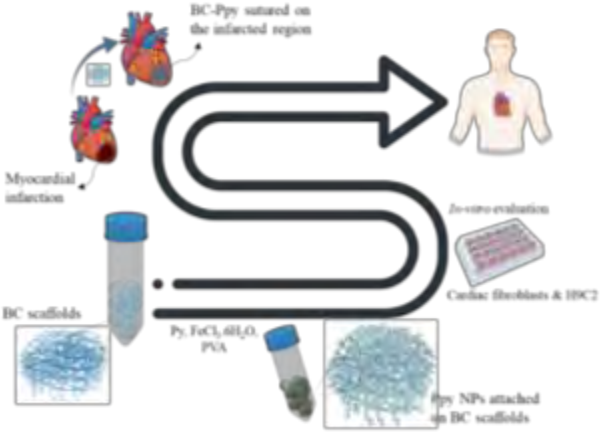
BC-Ppy sutured on the infarcted region
Myocardial infarction
In-vitro evaluation
Cardiac fibroblasts & H9C2
BC scaffolds
Py, FeCl$_3$.6H$_2$O, PVA
Ppy NPs attached on BC scaffolds

Magnetic responsive hydrogels for neural regeneration

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Spinal cord injuries affect 2,000,000 people worldwide. However, an effective and definite treatment does not exist yet due to the complexity and limited regeneration potential of the central nervous system. For this reason, developing new regenerative approaches is required.
With that aim, we initiated the exploration of some new strategies involving hydrogels derived from natural polymers and magnetic iron oxide nanoparticles, considering their attractive properties for biomedical applications1,2,3.

On the one hand, magnetic nanoparticles were coated with hydrogels (e.g. chitosan and hyaluronic acid). For chitosan coating, ionic gelation with sodium tripolyphosphate (non-toxic polyanion) was used. Whereas for hyaluronic acid coating, only incubation and sonication were required. On the other hand, natural hydrogels were obtained by lyophilisation of polymer solutions containing the selected magnetic nanoparticles. The coated particles present high colloidal stability, while hydrogels were porous with superior mechanical properties in the case of collagen hydrogels. Preliminary cell assays with primary neural cells showed high cell viability in collagen and gelatin hydrogels and chitosan and hyaluronic acid coated nanoparticles.

To sum up, natural hydrogels and nanoparticles coated with natural polymers seem to arouse a positive response in primary neural cells. Nonetheless, some of their properties need to be optimized and further research on cell responses is needed to confirm the actual regenerative potential of these biomaterials

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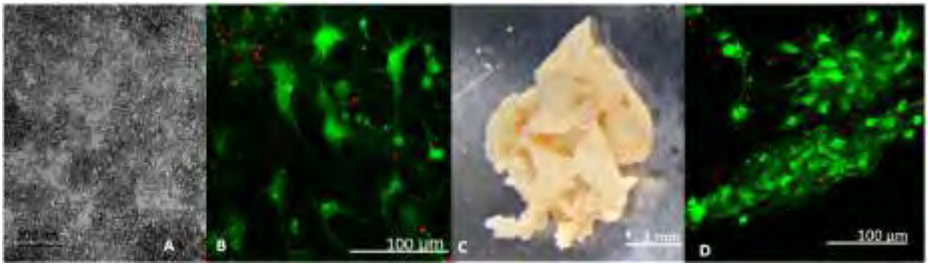

Figure 1: a) Magnetic nanoparticles; b) Primary neural cells after 24h of exposure to 0.1 mg/mL of chitosan coated nanoparticles; c) collagen hydrogel with nanoparticles; and d) neural cells cultured on the collagen hydrogel. Alive cells stained with calcein (green) and dead cells with ethidium homodimer 1 (red).

Current-induced control of chiral magnetic textures in magnetic insulators

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The use of the spin of the electrons in devices is having a tremendous impact on our electronics and computing technologies. Tell-tale examples are found in the electric switching and reading of magnetic tunnel junctions as well as in the controlled displacement of domains and domain walls in magnetic thin films. Despite the enormous progress that has been made, current devices are restricted to the use of metallic ferromagnets, which typically suffer from high losses and are limited in frequency.

Magnetic insulators (MIs), such as rare earth garnets ($R_3Fe_5O_{12}$; R=Y, Tm ,..), have attracted a lot of interest because of their low Gilbert damping and high-frequency dynamics. Although being electrically insulating, MIs can couple to spin currents, making thus possible to employ these materials as active elements in electronic devices.

In this talk, we show how we can stabilize chiral domain walls and skyrmions in $Tm_3Fe_5O_{12}$ (TmIG) coupled to Pt and manipulate them by proximity electric currents (Fig. 1) [1,2]. We demonstrate the chiral nature of the domain walls and skyrmions via nitrogen-vacancy magnetometry and investigate their dynamics driven by current pulses. We find that the domain walls in TmIG exhibit mobilities comparable to those achieved with metallic ferromagnets and reveal that the dynamics of the skyrmions are governed by the ferrimagnetic order of the4 crystal and pinning, resulting in a large skyrmion Hall effect characterized by a negative deflection angle and hopping motion. Further, we show that the mobility of the walls and skyrmions can be modified by exchange coupling TmIG to an in-plane magnetized $Y_3Fe_5O_{12}$ (YIG) layer, which distorts the spin texture of the magnetic nanostructures leading to a directional-dependent rectification of their dynamics. This effect, which is equivalent to a magnetic ratchet, is exploited to control the flow of domain walls and skyrmions in devices.

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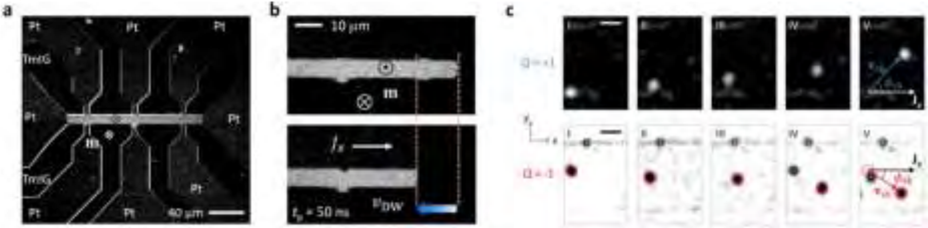

Figure 1: **a**, Magneto-optical Kerr effect (MOKE) image of a TmIG/Pt device showing current-induced switching of TmIG (bright region). **b**, Demonstration of current-driven wall motion. A current pulse $J_x \sim 10^{12}$ A m^{-2} in Pt drives the walls in TmIG at velocities v_{DW} of 300 m/s. **c**, MOKE images showing the displacement of skyrmions in YIG/TmIG/Pt following a sequence of current pulses. The topological charge of the skyrmions (*Q*), which can be controlled by the orientation of the skyrmion core (bright/dark), results in a transverse deflection of the skyrmions.

Frequency shift approximation in simulations of HR-AFM images with a CO-functionalized tip

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Image simulations of High-Resolution Atomic Force Microscopy with a CO-functionalized tip have greatly improved as we better understand the theory of such images [1,2,3]. Models such as the FDBM allow us to calculate the tip-sample interaction force (F_{ts}) in a sizable $3D$ space. Nevertheless, AFM experiments can only directly measure changes in the tip's oscillation frequency (frequency shift, Δf). So, to properly compare simulated AFM data to real-world experiments, we must further change the theoretical F_{ts} to a theoretical Δf [4]. The straightforward way to achieve this is to integrate the F_{ts} numerically, along the complete length of the tip oscillation, as described in [5]. However, this method requires the F_{ts} to be calculated at many different points along the z-axis, making the calculations grow considerably. An option that avoids this inconvenience is approximating the Δf with the force gradient ($\nabla_z F_{ts}$) calculated at a single point in the z-axis, which works well for the small oscillations in tuning force AFM. Still, different HR-AFM experiments have oscillations between 0.2 and 1Å, where the force gradient approximation may not hold.
For the last case, we futher propose a F_{ts}-based Δf approximation, considering the force at the point of the closest approach of the tip. Meanwhile, the $\nabla_z F_{ts}$ approximation, only considers the mean average position of the tip through a complete oscillation cycle. With FDBM [1], we then simulated the HR-AFM data of different experimentally-relevant molecules (such as trimesic acid [6], pentacene, and pyridine) and calculated the Δf with the three methods previously described. We observed that the integral function and the F_{ts} approximation have similar results, but the $\nabla_z F_{ts}$ approximation does not, as shown in Fig. 1. The difference comes from the CO tip relaxation, as the shape of the force curve changes in a few fractions of an Å due to the CO molecule's deflection. So using the $\nabla_z F_{ts}$ approximation does not fare well because the data of the average plane of the oscillation does not relate to the data at the point of closest approach. In conclusion, the proposed force approximation yields very similar results to the complete integral. Also, it has the advantage that it does not require a wide range of ts distances to approximate the Δf.

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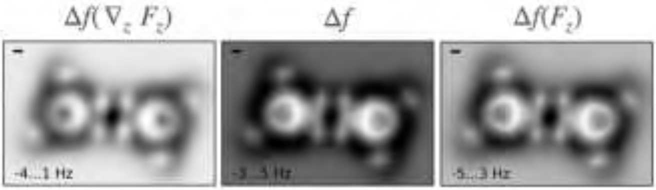

Figure 1: Theoretical frequency shift approximations of a trimesic acid dimer, where carboxyl groups form a double H bond. (left) Approximation based on the force gradient at the mean tip--sample distance, (center) exact calculation as the integral of force versus distance curves, (right) approximation based on the force at the distance of closest approach. Tip-sample distance is 3.17Å, amplitude is 0.55Å, scalebar length is 1Å.

Three-dimensional interconnected anodized aluminum oxide (3D-AAO) metamaterials using different waveforms and metal layers for RGB display technology applications

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Research into the artificial reproduction of vibrant colours in natural creatures and the reproduction of their structural colours has generated considerable interest. One inorganic material that has been studied for the generation of these artificial colours is anodic aluminium oxide (AAO)[1-2]. For example, 3D anodic aluminium oxide (3D-AAO)[3-4] metamaterials act as distributed Bragg reflectors. This study examines the effect of the application of various waves (square, sinusoidal, and sawtooth) during the generation of 3D-AAO on the optical and morphological properties of these 3D metamaterials. The effect of the waveform in the colours and hues have been explained by a theoretical model. Furthermore, the work analyses how colour can be improved by depositing a thin metal layer on top, obtaining, from a simplistic point of view, a combination of two effects: A Bragg reflector (3D-AAO) and an optical reflector (metal mirror). For that, different metals like Au, Pt, and Cr have been studied. The thickness of the metal layer has been theoretically modelled[5]. This study paves the way for a new approach to developing structural colours for their use in for example RGB display technologies.

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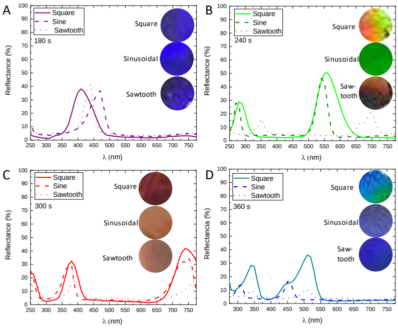

Figure 1: UV-Vis reflectance spectra as a function of the wavelength of 3D-AAO nanostructures or different waves and rest times. (a) 180 s, (b) 240 s, (c) 300 s, and (d) 360 s. In the inset, optical images of 3D-AAO colour for different waves and resting times were studied.

Extraordinarily transparent compact metallic metamaterials

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Abstract

Metals are highly opaque, yet we show numerically and experimentally that densely packed arrays of metallic nanoparticles can be more transparent to infrared radiation than dielectrics such as germanium, even for arrays that are over 75% metal by volume. Despite strong interactions between the metallic particles, these arrays form effective dielectrics that are virtually dispersion-free, making possible the design of optical components that are achromatic over ultra-broadband ranges of wavelengths from a few microns up to millimetres or more. Furthermore, the local refractive indices may be tuned by altering the size, shape, and spacing of the nanoparticles, allowing the design of gradient-index lenses that guide and focus light on the microscale (see figure a). The electric field is also strongly concentrated in the gaps between the metallic nanoparticles, and the simultaneous focusing and squeezing of the electric field produces strong 'doubly-enhanced' hotspots (see figure b) which could boost measurements made using infrared spectroscopy and other non-linear processes over a broad range of frequencies, with minimal heat production.

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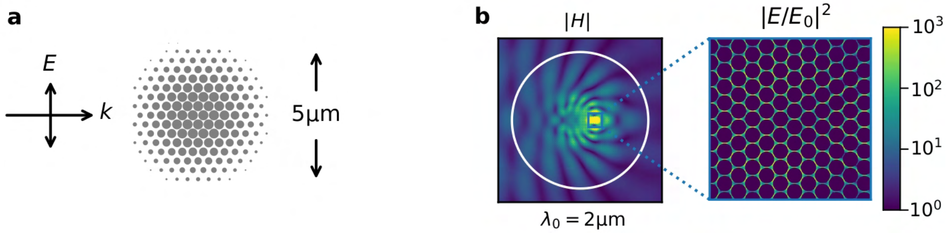

Figure 1: (a) Schematic of a 'concentrator' gradient-index lens composed of gold nanocylinders on a triangular lattice with 50nm site-to-site separation (b) Magnetic near-fields and broadband 'doubly-enhanced' electric field hotspots

Composite cathode for Li-sulfur system: Effect of inorganic additives on electrochemical performance

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Abstract

The rapid development of portable electronic devices together with new large-scale applications stimulate demand for battery systems providing high capacity and energy density. Since the classical Li-ion batteries based on intercalation approached their limits, researchers have moved their attention to a Li-sulfur battery with a theoretical capacity of 1675 Ah kg^{-1} and energy density of 2600 Wh kg^{-1}. Except for the non-conductivity of elemental S and large volume changes during redox reactions, the main problems are related to the dissolution of lithium polysulfides (PS) in the electrolyte. PS diffusion to the anode compartment of the Li-S battery causes severe redox shuttle between the cathode and Li anode and results in a low coulombic efficiency for charging/discharging and a fast self-discharge during storage[1]. Non-conductivity of sulfur requires the incorporation of electron-conductive additive and volume changes accompanying PS formation represent a challenge for cathode architecture. The carbonaceous materials were demonstrated to enhance the performance of sulfur-based cathode composites. In addition, the inorganic component provides a higher adsorption ability for PS. In our work, we studied the influence of two different activated carbons (Fluka or Penta) and five inorganic additives on the electrochemical performance of the sulfur composite cathode. The electrochemical behavior of the materials was evaluated by cyclic voltammetry at 0.1 mV s^{-1} and galvanostatic chronopotentiometry and correlated with their morphology. The inorganic additives (nano-TiO_2, TiO_xN_y-anatase, rutile/TiO_xN_y, P90, $Li_4Ti_5O_{12}$) in the cathode increase the capacity of the corresponding Li-S cell. This increase is more pronounced for Penta carbon with a larger external surface area of 345 m^2 g^{-1}. Commercial P90 titania in the Penta/sulfur composite cathode provides the highest voltammetric charge capacity of 731 mAh g^{-1}. This effect is ascribed to the excellent polysulfide adsorption ability of this disperse material. TiO_xN_y-anatase additive exhibits the second-highest capacity improvement due to surface-enhanced redox chemistry of its conductive and sulphiphilic surface. The electrochemical performance of all the Li-sulfur cells containing Penta/sulfur/inorganic additive cathode is boosted by the separator modification with P90. The best performance provides the cell containing Penta/sulfur/nano-TiO_2 cathode and P90-modified separator. The synergic effect of the Penta carbon large external surface area, the high surface area of nano-TiO_2 boosted by the presence of highly disperse P90 in the separator manifests itself by the voltammetric charge capacity of 881 mAh g^{-1}.

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POSTERS

Process optimization for quality-oriented manufacturing of lipid nanocarriers

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Introduction. Lipid nanoparticles (LNPs) have gained great attention in research as nanocarriers for targeted drug delivery mainly due to their unique properties, such as high bioavailability, enhanced drug solubilization and protection, and biocompatibility. Here we focused on developing optimal LNPs as advanced drug delivery systems for improving the encapsulation of hydrophobic drugs.

Methods. We used "Design of Experiments" approach for screening of main formulation parameters influencing responses, this way, we elaborated several LNPs according to DOE by using the solvent injection technique (Figure 1). We evaluated mean particle size, polydispersity index (PDI) and zeta potential (ZP) by dynamic light scattering and electrophoretic mobility. One optimal composition computationally predicted was then prepared and its stability was studied upon storage at different temperatures (4ºC/RT).

Results. Most of the formulations engineered resulted in appropriate physical properties, with small hydrodynamic sizes and narrow size distribution. In addition, optimized LNPs were stable over time at both temperatures tested. From the initial batch volume, we were able to scale-up the reaction leading to the formation of optimal LNPs without observing changes in the physicochemical characteristics of LNPs obtained, thus confirming their high stability and scalability of the process.

Conclusions. We have successfully engineered optimal LNPs in a first panel of formulations with different characteristics ready to be used as drug delivery systems. The efficacy of these optimized LNPs as nanocarriers will be tested soon.

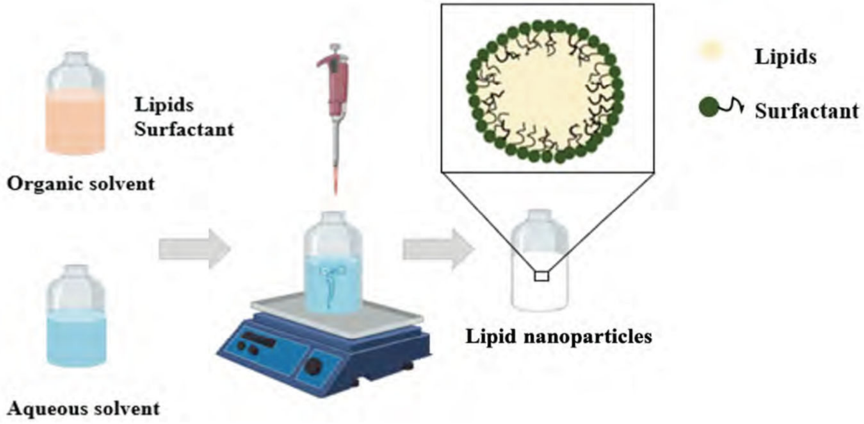

Figure 1. Lipid nanoparticles production by solvent injection technique.

IRRADIATION OF GOLD NANOPARTICLES WITH ULTRA-FAST LASER PULSES

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Abstract Gold nanorods (NRs), pseudo-one-dimensional rod-shaped nanoparticles (NPs), have become one of the burgeoning materials in the recent years due to their anisotropic shape and adjustable plasmonic properties [1]. Under light irradiation, noble metal nanoparticles, particularly those characterized by localized surface plasmon resonance, commonly known as plasmonic nanoparticles, generate a strong electromagnetic field, excited hot carriers, and photothermal heating. The irradiation of rod–sphere assemblies with ultrashort laser pulses, producing structures that are very difficult to obtain by other methods [2]. The optical response of these assemblies displays several peaks arising from the interaction of the plasmon modes of the individual particles, offering thus great flexibility to control the energy deposited on the individual particles. Judicious selection of the wavelength and fluence of the laser pulses allows fine control over the changes produced: the particles can be melt and/or the organic bonds cleaved. In this way, it is possible to generate structures "à la carte" with a degree of control unmatched by other synthetic protocols. The method is exemplified with gold nanoparticles, but it can be easily implemented on particles composed of different metals, widening considerably the range of possibilities. The final structures are excellent candidates for surface-enhanced spectroscopies as they have a very intense electric field located outside the structure, not in the gaps.

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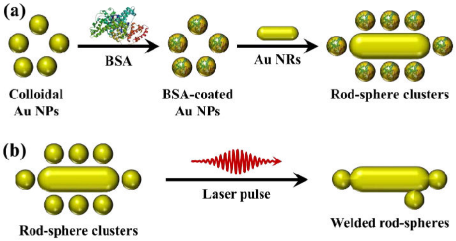

Figure 1: **Schematic representation of (a) synthesis of Au rod– sphere nanoclusters and (b) welding of those nanoclusters by irradiation with fs laser pulses.**

Time resolved study of living cells transference by BA-LIFT

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Blister Actuated - Laser-Induced Forward Transfer (BA-LIFT) [1], is a disruptive technique in the bioprinting field through which a wide variety of bioinks can be printed preserving cell integrity. BA-LIFT has been used to print several types of cells. All of them exhibit an extremely high cell viability meanwhile their metabolic capacities remain unaltered. The use of a polymeric intermediate layer, main characteristic of the BA-LIFT approach, creates a smooth transference process mediated by a blister formation. The deformation of the intermediate layer into a blister pushes forward the bioink forming a jet that collapses generating a droplet. We have been able to successfully develop a numerical FEM-CFD to study the transference process.
Our approach [2], uses a thick intermediate layer made of a commercial adhesive polyimide tape which protects the bioink from the upcoming laser radiation. This approach not only eases the donor preparation due to its simplicity but also enables real time image acquisition due to its transparency in the visible range. Top and side viewing systems can be attached to the transference set-up, allowing us to track cells down during the whole transference process.

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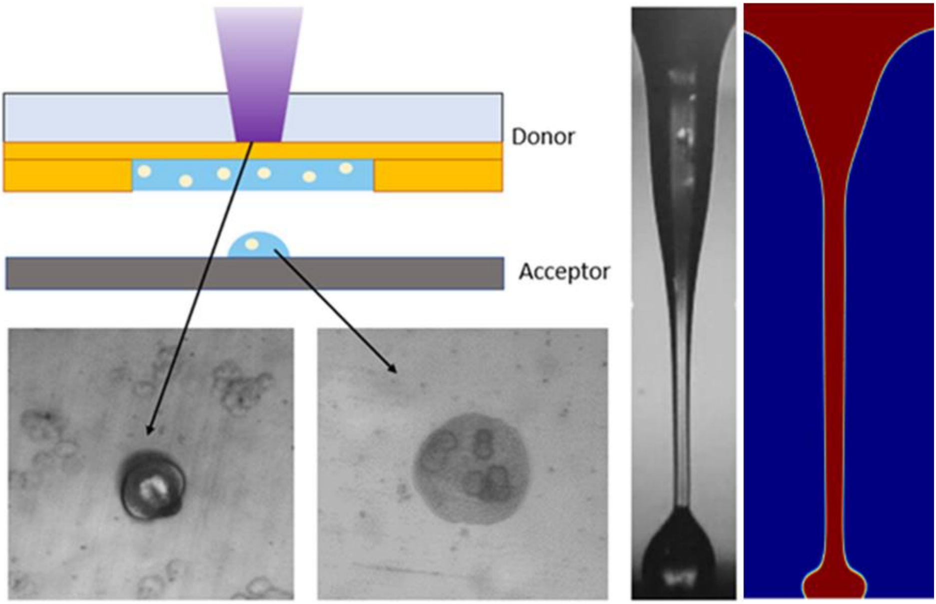
Graphical abstract



Plasmon Optomechanical Switch

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In this work we theoretically demonstrate the use of a two-level optomechanical system actuated by plasmon-mediated optical forces as a reconfigurable nanophotonic switch. We have simulated a nanostructured suspended gold membrane allowing the normal excitation of a Surface Plasmon Polariton by patterning an air nanohole array [1]. By placing the membrane in the proximity of a reflecting substrate assembling a Fabry-Perot microcavity, we enter the strong coupling regime, obtaining a mode splitting which provides two stable mechanical states, accessible by tunning the illuminating wavelength [2]. It is also possible to dynamically actuate on the length of the cavity by introducing a mechanical actuation on the membrane by means of an induced harmonic displacement. The oscillatory movement of the suspended membrane can be manipulated via optomechanical amplitude modulation (cooling or amplification). The final stable state of the dynamical system can then be actively chosen, opening the door for the development of an optomechanical switch [2].

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Figures

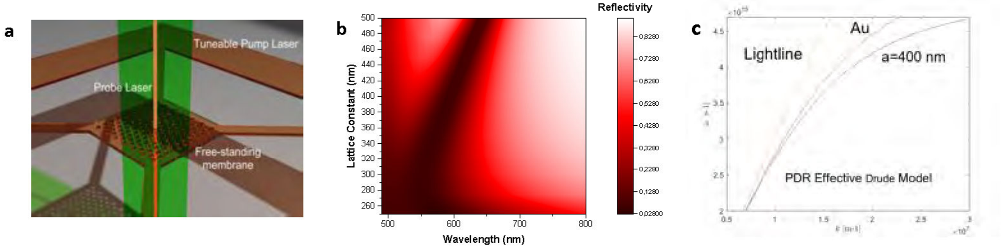

Figure 1: **a**. Schematic depiction of the optomechanical system. **b**. Color map of the membrane reflectivity as a function of the lattice constant of the nanohole arrays and the illuminating wavelength. The excitation of the Surface Plasmon Polariton is viewed as a reflectivity drop. **c**. Surface Plasmon dispersion relation calculated by an Effective Drude Model.

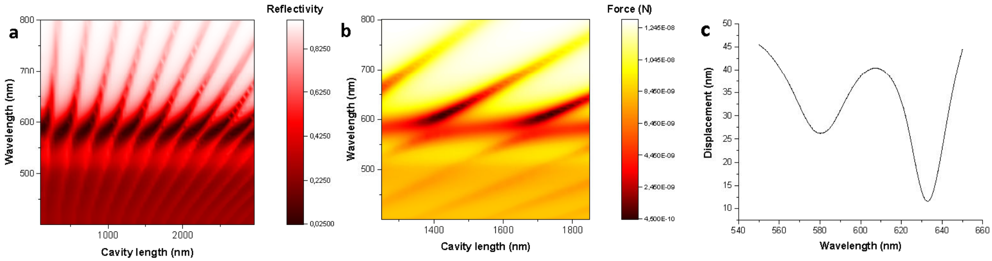

Figure 2: **a.** Reflectivity (in color) as a function of the illuminating wavelength (y-axis) and the cavity length (x-axis). **b.** Optical Force calculated as a function of the wavelength and the cavity length. **c.** Relative mechanical displacement of the mechanical structure placed 1500 nm over the reflecting substrate as a function of the wavelength of the pump laser.

Integrated nano-opto-fluidic platform for nanoparticle characterization in liquid

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Last years have witnessed an increasing interest in the development and active control of the mass transportation at the nanoscale, which has potential applications in many different areas ranging from biological sensors to environmental control. In this sense, photonic crystal sensors have been revealed as very promising candidates due to their versatility, integration capabilities and high sensitivity. The patterning of a periodic air hole array in a dielectric material opens a bandgap in the light propagation through the structure via Bragg reflection. Within this bandgap it is possible to engineering a defect, allowing the confinement of the light at a desired wavelength, which depends on the effective refractive index of the materials. Here, we propose the design of a nanochannel made by the side coupling of two one-dimensional photonic crystal nanobeams. A liquid flowing in between the two nanobeams modifies the effective refractive index of the whole system, consequently shifting the optical resonance. We theoretically demonstrate the high sensitivity of the system to detect refractive index changes (reaching a value of 10^{-6}). This work opens the door for novel applications as the detection of nanoparticles in liquid.

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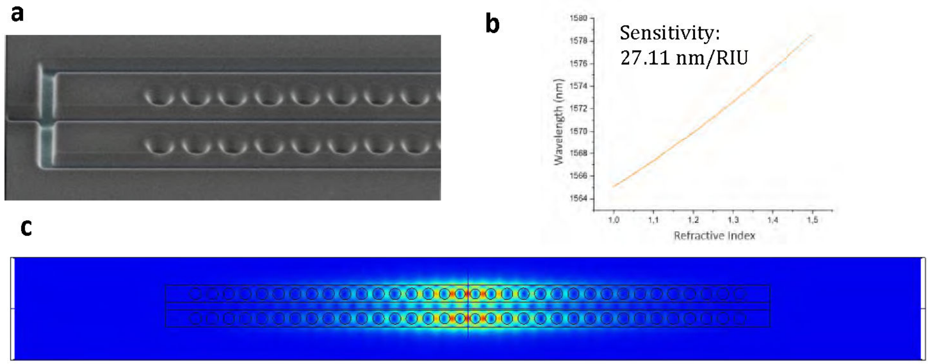

Figure 1: a) Double nanobeam photonic crystal containing channels for liquid sample deposition. (b) Cavity mode's wavelength as a function of refractive index. (c) Double nanobeam simulation of eigenmode.

Efficiency Of Different Size Gold Nanorods For Optical Hyperthermia

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Introduction: Conventional treatments such as chemotherapy, radiotherapy, and surgery are the most common cancer therapies. Optical hyperthermia (OH), also called photothermal therapy, is an emerging cancer therapy [1][2] that uses gold nanoparticles to destroy the tumor cells by selectively increasing the temperature inside the cells when irradiated with a laser at an appropriate wavelength. Gold nanorods (GNRs) are capable of targeting cancer cells when biofunctionalized with molecules specifically overexpressed in cancer cells [2]. This work focuses on the elimination of tumor cells by OH in the presence of GNRs of different sizes using glioblastoma (CT2A) and melanoma (B16F10) cell lines as models, aiming to determine the best performing size.

Material and methods: In order to determine the efficiency of different sized GNRs, commercial GNRs (10x41nm), and experimental nanorods (10x40nm and 20x65nm, coated with PEG) were evaluated. CT2A and B16F10 cells were seeded at 7.000 cells/well on P96 multiwell plates. One day after seeding, GNRs were added at 2 µg/mL and then incubated for 24h. Cell cultures were then irradiated with a laser at 808nm and 4,5W for 10 min. Cell viability was determined by XTT assay and by calcein-propidium iodide staining.

Results: Heating curves after laser irradiation and cytotoxicity tests at different GNR concentrations were performed for each type of GNR in order to optimize both parameters to perform the OH. Tumor cells were eliminated when irradiated at 4.5W for 10 min in the presence of all types of GNRs at 2 µg/mL. The cell mortality obtained was high for both cell lines, being 80-90% for CT2A and 50-60% for B16F10 (Figure 1 and 2).

Conclusion: All the GNRs tested resulted as optimal nanoparticles for photothermal therapy applications, with the 20x65 nm GNRs being the most efficient, producing the highest percentage of cell death.

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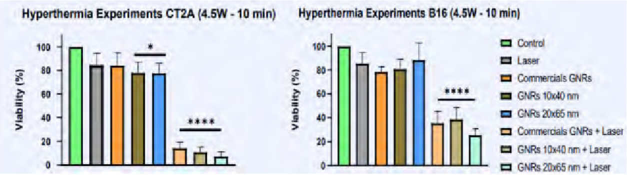

Figure 1 and 2: Cell viability of different conditions in a hyperthermia experiment (Laser, GNRs and GNRs + laser) in CT2A and B16F10. The bars represent means ± SEM of three independent samples performed in triplicate. Statistically significant differences determined by One way - ANOVA are represented: (*) p<0,05, (****) p<0,0001.

Preparation and characterization of functional bio-nanocapsules via solvent/nonsolvent methodology

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Abstract

Climate protection, reduction of greenhouse gas emissions and saving of fossil resources are key elements for a more sustainable future. The transformation of biobased materials to the nanoscale is a very primising approach to this challenge, providing them with new properties required in many sectors, but they must offer functional properties for high-volume applications and better performance than fossil-based materials to be accepted by the industry and end users. [1]

Lately, the increasing concern of the application of inorganic nanoparticles for antimicrobial activity due to their toxicology, is driving scientists to move towards the fabrication of non-toxic, biocompatible and biodegradable nanocapsules, in several sectors. [2] As such, the authors developed functional nanocapsules from cellulose acetate polymer and tea tree oil as bioactive compound in order to obtain a natural nano-additive for the antimicrobial and antioxidant functionalities. These nanocapsules were prepared by the nanoprecipitation method using environmentally safe solvents and were characterized by the appropriate techniques.

These developments were performed in the scope of the Bionanopolys project that intends to strengthen the circularity of nano-enabled bio-based materials in the economy launching and promoting an open innovation test bed to develop innovative bionanocomposites from main feedstocks in Europe and bio-based nanoproducts in relevant sectors and improving technologies and processes in different pilot lines. This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under grant agreement Nº 953206.

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Graphene-based electrodes for non-conventional crystalline silicon solar cells

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Graphene is considered as a promising candidate for the new emerging generation of transparent electrodes to be used in many applications such as displays, touch screens and/or solar cells [1, 2]. Its unique mechanical, electrical and optical properties make it a relevant material in a near future [3]. In this work, a new design of transparent conductive electrode based on a graphene monolayer is evaluated by its incorporation into non-standard high-efficiency crystalline silicon solar cells, where the conventional emitter is replaced by a MoOx selective contact. The device characterization reveals a clear electrical improvement when the graphene monolayer is placed as part of the electrode. The current–voltage characteristics of the solar cells with graphene shows a higher FF and V_{oc} thanks to the improved sheet resistance. Figure 1 shows the electrical conductance maps acquired on das-Nano Onyx, using reflection-mode terahertz time-domain spectroscopy (THz-TDS), where the measurable frequency range analysed was from 0.1 THz to 5 THz. Improved conductance values of around 4.5 mS are achieved for the graphene-based electrode, in comparison with 3 mS, for bare ITO. These results so far clearly open the possibility to achieve a noticeably improvement in the contact technology and therefore to further enhance non-conventional photovoltaic technologies.

Acknowdlegments: This research has been supported by Grants PID2019-109215RB-C41 and PID2019-109215RB-C42 funded by MCIN/AEI/ 10.13039/501100011033

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Figures

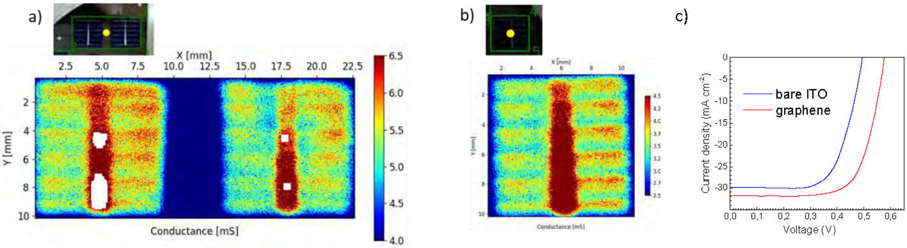

Figure 1: THz-TDS Conductance maps obtained for the solar devices. The areas in between the fingers have conductance around a) 4.5-5.5 mS (sample with graphene monolayer) and b) 3-3.5 mS (sample with bare ITO). The lines of higher conductance correspond to the metallic fingers. c) Compared electrical characteristics of the solar cells with bare ITO and adding a graphene monolayer.

Functionalized silicon microdevices for sulforhodamine and doxorubicin pH-controlled release in HeLa cells

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The development of micro/nano-drug delivery systems (DDS) has attracted the attention of researchers seeking stimuli-controlled delivery at an intracellular level. Acidic microenvironment of tumours could be an interesting trigger signal. In the present work we study silicon microdevices functionalized with doxorubicin (DOX, chemotherapy DNA-intercalating drug) or sulforhodamine B (SR, fluorescent probe) as an intracellular DDS in HeLa cells and analyse the release of these drugs in response to external pH. Our results showed a higher drug release at acidic pH of both molecules, SR and DOX.

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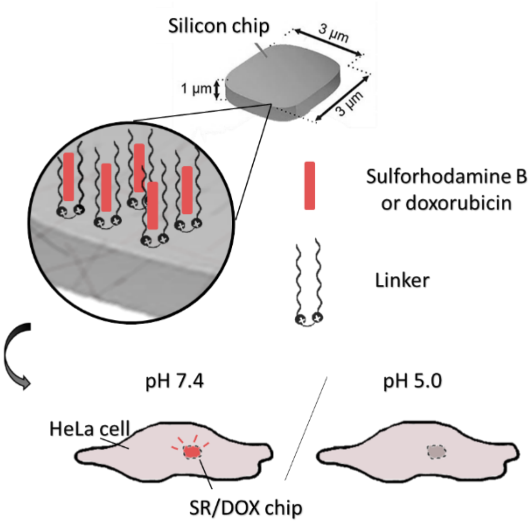

Effect of temperature reactor in the clays gas-phase modification with silanes

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Abstract

It is well known that the incorporation of nanoclays into polymeric matrices improves their mechanical, thermal and barrier properties. However, it is essential to functionalise the surface of the nanoparticles to achieve optimal blending. In this sense, BIONANOPOLYS [1] is a project that joins European experts in the field of bio-based nanoscale materials which scope is not only the development of novel functionalisation methods, but also to upgrade the pilot plants dedicated to the modification of nanoparticles according to the applications defined by industry specifications. Therefore, this research aims to study the modification of commercially available montmorillonite (MMT) and layered double hydroxides (LDH) with 3-aminopropyltriethoxysilane (APTES) and tetraethyl orthosilicate (TEOS) in gas-phase.

In the experiments, a certain amount of MMT and LDH are introduced into each of the porcelain vessels, while either TEOS or APTES are placed in the bubbler and heated to a given temperature. Argon is then introduced into the bubbler, allowing the modifier to be fed into the quartz reactor where the reaction takes place. To analyse the effect of reactor temperature in the modified clays, the previous process is carried out at four different temperatures. The obtained nanomaterials are characterised by means of TGA, FTIR, XRD, and laser diffraction techniques.

The results obtained show that it is attainable to modify the surface of clays by treatment with silanes in gas-phase. By controlling the temperature, it is possible to tune up the degree of surface functionalisation, making feasible to change the hydrophobicity of the materials, improving the interaction between the nanoclays and the polymeric matrix.

This work is supported by the European Union-Horizon 2020 (BIONANOPOLYS-H2020-NMBP-TO-IND-2018-2020 - Nº 953206).

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Figures

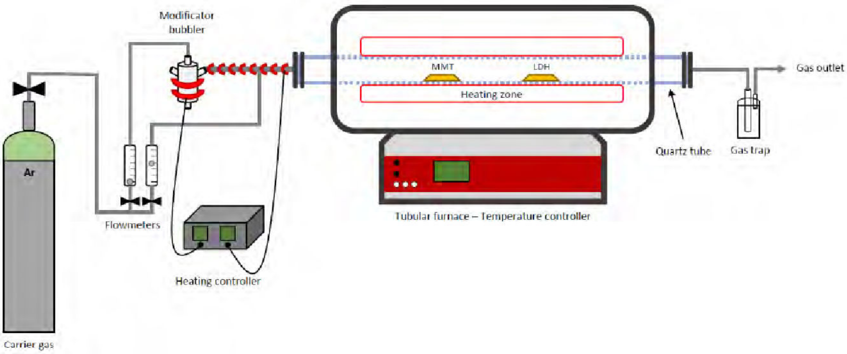

Figure 1: Scheme of tubular furnace experimental situation

Hexon-modified icosahedral gold nanoparticles as surrogates for adenovirus

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We present the preparation of surrogate adenovirus particles, which comprises generating icosahedral gold nanocores functionalized with a polyethylene glycol (PEG) layer, and subsequently decorated with hexon protein – the most abundant surface protein of Adenovirus Serotype 5 (Adv 5). Thus, this study addresses three highlight aspects: 1) The preparation of gold nanoparticles (AuNPs) with perfect icosahedral shape in a size range similar to the dimensions of Ad 5; 2) the development of a protocol ensuring homogeneous surface coverage of AuNPs with different types of functional PEGs; and 3) both covalent and non-covalent anchoring of hexon protein at the surface of pegylated icosahedral AuNPs.

The potential of the hexon-modified icosahedral AuNPs to act as surrogates for Adv 5 was evaluated by studying their interaction with a hexon protein-selective polymer. Only AuNPs with hexon protein on their surface bound to this selective polymer as real Adv 5 is expected to do, demonstrating that they are available to be used as surrogate synthetic viruses.

Polystyrene-modified magnetic nanoparticles as Pickering stabilizers

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We present here the preparation of switchable water-in-oil (W/O) and oil-in-water (O/W) Pickering emulsions with a polar solvent (as oil phase) only stabilized by polystyrene-modified magnetic nanoparticles. Initially, the ability to form Pickering emulsions of bare magnetic nanoparticles was evaluated concluding that they were not able to form W/O Pickering emulsions. For this reason, a new coating methodology based on the radical polymerization of a hydrophobic polymer (polystyrene) on the nanoparticle surface have been developed in order to modify the wettability of the bare magnetic nanoparticles. In this way, stable W/O and O/W Pickering emulsions were achieved being possible to continuously switch from one to other by changing the water/oil phase ratio. All variables related to the formation and stability of the Pickering emulsions were also studied and optimized. It should be noted the high stability in terms of temperature, pH and ionic strength as well as the easy and reproducible preparation of these emulsions.

$HoPO_4$ bioprobes to increase contrast in ultra-high field MRI scanners

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Currently, magnetic resonance imaging (MRI) is one of the most widely used bioimaging techniques for clinical diagnostic. To increase the sensitivity of MRI and, therefore, achieve a more accurate diagnosis, contrast agents (CAs) consisting of Gd^{3+} complexes or superparamagnetic iron oxide nanoparticles (NPs) can be used. Another strategy recently suggested for this purpose, and which is in the experimental stage, is the use of more powerful magnetic fields than those used in the clinic. Unfortunately, the mentioned CAs are not efficient at these high fields so it is necessary to develop new CAs for UHF (ultra-high field) scanners. In this work, we propose the use of holmium phosphate ($HoPO_4$) nanoparticles, due to the high magnetic moment of Ho^{3+} cation [3], and the low water solubility and high biocompatibility of lanthanide phosphates [2]. In order to demonstrate the suitability of such NPs as CAs for UHF MRI, we first describe a method based on a precipitation reaction in polyol medium to synthesize uniform $HoPO_4$ nanocubes (Fig. 1a) with variable size (27, 48 and 80 nm). A procedure for coating them with polyacrylic acid (PAA) to avoid their aggregation in physiological medium, which is a requirement for *in vivo* applications, is also described. Subsequently, the transverse relaxivity (r_2) at ultra-high field (9.4 T) of aqueous suspensions of the obtained NPs is analyzed as a function of the NPs size in order to determine the optimum CA, which turned out to be the one presenting a size of 48 nm. A biocompatibility study of these NPs is also presented, showing the absence of toxicity of these NPs, which is also an essential requirement for their *in vivo* application. Finally, MRI images of different organs of a mouse obtained by UHF MRI in the presence of these $HoPO_4$ NPs are shown (Fig. 1b), demonstrating their potential usefulness as contrast agents for this medical diagnostic technique [1].

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Figures

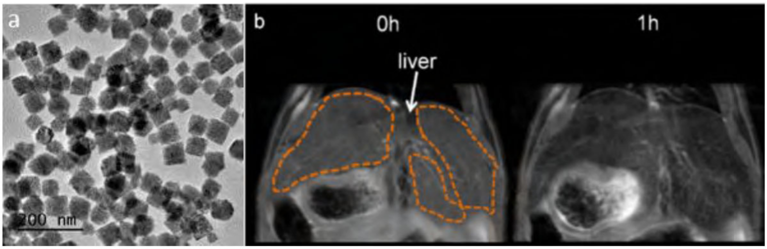

Figure 1: a) TEM micrograph of $HoPO_4$ NPs and b) representative T2-weighted MR images before and after the intravenous injection of such NPs.

Response of different nanaparticles on a biosensor based on IODM

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The Interferometric Optical Detection Method (IODM) is characterized by the use of two interferometric signals, employing two interferometric measurements: a first interferometric optical reference, and a second interferometric signal measurement observed in the sensing region of the signal interferometer. In this way, the optical reading system converts the changes caused by optical transduction into a unique and sensitive detection variable. The interferometers used are based on Fabry-Perot-based interferometers that act as biotransducers. In the present work, the signals obtained from magnetic nanoparticles coated with antibodies on these sensor surfaces are shown, with the aim of increasing the signal obtained with respect to the use of antibodies incubated directly.

Multimodal detection of atherosclerosis using Solid Lipid Nanoparticles

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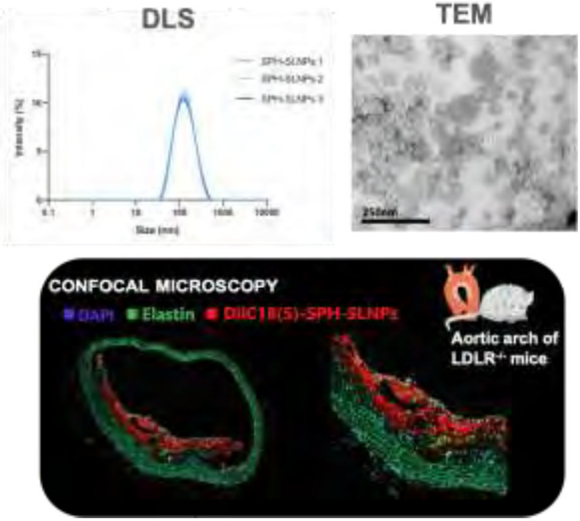
Atherosclerosis and its clinical complications are major constraints to living long and healthy lives. Therefore, tools capable of measuring disease activity are necessary. During this work, Solid Lipid Nanoparticles (SLNPs), a type of NP that is formed by a solid lipid core matrix and that is stabilized using surfactants, were synthesized as potential contrast agents for atherosclerosis. For that purpose, the enzyme driven accumulation of Sphingomyelin (SPH) in the atherosclerotic plaque was exploited.

SLNPs have been produced using Sphingomyelin (SPH) as the main lipid and cholesterol as the stabilizer. They were synthesized using the Solvent Injection Method. In this method, surfactants and lipids are solubilized in a semi-polar water miscible solvent. Afterwards, this organic phase is rapidly injected, under constant stirring, into an aqueous phase. As a result, organic solvent distributes rapidly into the aqueous phase and SLNPs are formed. After thorough sample characterization, the accumulation of the SPH-SLNPs in atherosclerotic plaques was evaluated with ex vivo fluorescence imaging.

Hydrodynamic size distributions measured by dynamic light scattering (DLS) showed a narrow size distribution for all samples. In addition, TEM imaging also showed a narrow distribution of NPs. SPH-SLNPs showed aggregation when incubated with their specific enzyme Sphingomyelinase. Furthermore, ex vivo fluoresce imaging showed accumulation of the SPH-SLNPs in the aorta of LDLR-/- mice. These characteristics make SPH-SLNPs a suitable potential probe for pathophysiology and activity characterization.



Manufacturing of organ-on-a-chip devices based on glass,vinyl , and PDMS for cell and tissue culture

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An organ-on-a-chip is a microfluidic device capable of recreating a tissue or organ culture equivalent in a controlled micro/nanoenvironment, being able to simulate its dynamics, functionality, and/or physiological response. The main application of the organ-on-a-chip models is focused on the pharmaceutical industry to improve the safety and efficacy studies in the development of new drugs. This technology is also proposed as a future tool in the development of personalized medicine using patient-specific cells. This work presents a new organ-on-a-chip concept using vinyl for the generation of the microfluidic channels of the chip in combination with glass and polydimethylsiloxane [1,2].

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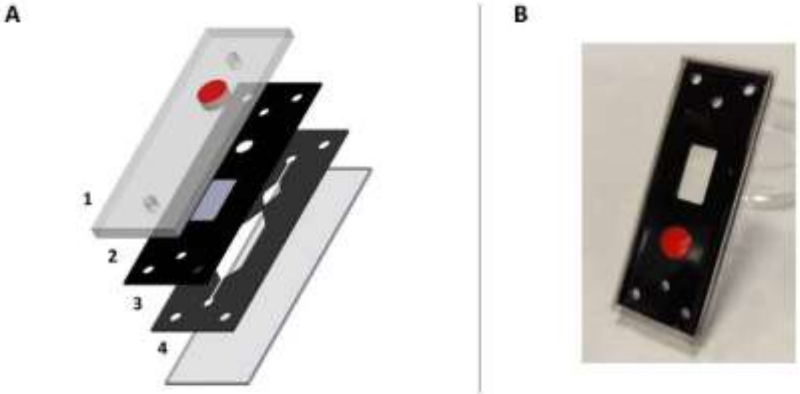

Figure 1: (A) 3D exploded view representation of the brain slice-on-a-chip (B) Picture of the final chip version employed for hippocampal slices culture. [2]

3D Skyrmionic configurations in soft magnetic nanodots with no Dzyaloshinskii-Moriya interactions

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Magnetic skyrmions are widely attracting researchers due to fascinating physics and novel applications related to their non-trivial topology [1]. Néel skyrmions have been extensively investigated in magnetic systems with Dzyaloshinkii-Moriya interaction (DMI) and Perpendicular Magnetic Anisotropy (PMA). However, so far, at least PMA is considered to be a necessary ingredient for skyrmion stabilization. In this work, Néel skyrmions were detected experimentally by using magnetic force microscopy techniques in Py sub-100 nm diameter nanoparticles (NP) [2]. This is a non-expected magnetization configuration in NP since the minimum energy configuration for these Py structures (without DMI and more remarkably, in absence of any magnetic anisotropy) is vortex state or single domain in plane magnetization [3]. In addition, we have used micromagnetic simulations to show that 3D quasi-skyrmions, spin textures with topological charge close to 1, can be stabilised in soft magnetic nanodots (planar disks and hemispheres) with no DMI. We have found that the range of geometrical parameters were the skyrmions are stabilized is wider in magnetic hemispheres than in planar circular nanodots [4]. We argue that the key factors responsible for the stabilization of DMI-free skyrmions are the magnetisation confinement and surface curvature. Besides, the curvature introduces chirality to the system, as the core magnetization direction and the radial magnetization component are coupled. We have calculated the state diagram for quasi-skyrmions as well as the 2D topological charges and gyrovector values, as a function of the geometrical parameters. Our results open the door for a new research line related to the nucleation and stabilization of magnetic skyrmions in a broad class of nanostructured soft magnetic materials.

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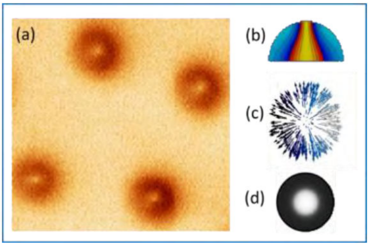

Figure 1:(a) MFM image of Py nanoparticles, (b) mz component of the magnetic configuration calculated by OOMMF (c) my component of the same simulation and (d) simulated MFM image corresponding to the same simulation.

Synthesis of Gold-Silver Chalcogenide Hybrid Systems through a New Synthetic Approach

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Developing alternative synthetic route for achieving nanoscale heterostructures can offer more structural and compositional diversities in the system, rather than those obtained by using traditional bottom-up approaches. In this work, a new synthetic route was developed for the synthesis of both Au-Ag_2Se and Au-Ag_2S hybrid systems by directly mixing Au and silver chalcogenides nanoparticles, instead of adding surfactant -Au(III) complexes [1,2] into Ag_2Se and Ag_2S nanostructured semiconductors. The results showed that the Au has partially fused with initial Ag_2Se and Ag_2S, resulting in the formation of two ternary interfaces ($AuAg_3Se_2$ and $AuAg_3S_2$) in between the metallic domain of Au and the initial Ag_2Se and Ag_2S, respectively. Their structures, chemical compositions and optical properties have been studied by electron microscopic techniques, X-ray diffraction and UV/vis spectroscopy. Furthermore, the DFT calculations were also performed to understand the relative thermodynamic stability of the phases involved in the process.

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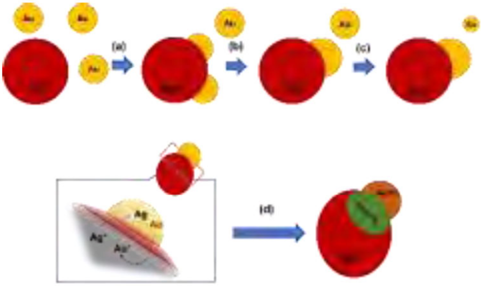

Figure 1: Schematic illustration of the heterodimer formation mechanism. a) NP heteroattachment, b) Au NPs coalescence at the chalcogenide surface, c) solution-mediate Au NPs ripening, and d) solid interface-confined galvanic replacement.

Specific immunoglobulins against sars-cov-2 in human samples and its validation with the elisa technique

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Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is an RNA virus responsible for the pandemic that started in March 2020 and caused over 2.1 million deaths worldwide. Therefore, it is necessary to test the majority of the population in a fast, cheap, easily, and reliable manner. In this work we report the development of a novel in vitro diagnostic system based on biophotonic sensing cells (BICELLs) (figure 1) [1-3] to detect specific immunoglobulins in serum and saliva against SARS-CoV-2. This system aims the label-free detection of anti-SARS-CoV-2 IgG, IgM, and IgA of patients testing PCR-positive (figure 1), using the interferometric optical detection method (IODM). The results obtained were correlated and validated with those obtained by ELISA observing a significant correlation between the two techniques.

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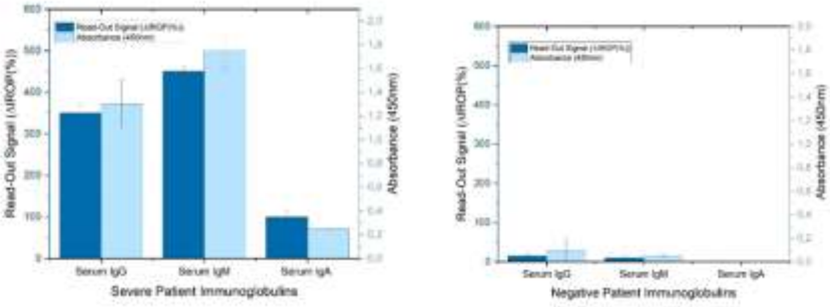

Figure 1: On the right are presented the results obtained for the antibody titers for a PCR-positive patient against SARS-CoV-2 measured by ELISA and IODM. On the left is the case of a negative patient.

Deposition of maleimide molecules on MoS2 under UHV conditions

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Nowadays there is increasing interest in performing controlled chemical reactions on van der Waals materials with several types of molecules to realize new multi-dimensional heterostructures, and open new pathways for different applications [1,2]. Recent studies demonstrated the successful covalent functionalization of transition metal dichalcogenides (TMDs) with different molecules [1,3,4]. One of these combinations is the covalent link between MoS2 monolayers and maleimide derivatives via “click” reactions [1,3,4] due to the soft nucleophilic character of sulfur. However, this synthesis is usually made under solution in liquid environments, and an ultra-high-vacuum (UHV) approach has not yet been attempted yet. In this work we deposit benzylmaleimide molecules on MoS_2 islands grown on a substrate of graphene/Iridium (111) under UHV conditions, and explore their adsorption on the surface by means of scanning tunneling microscopy (STM). Our results indicate that, rather than forming a covalent bond on the top Sulphur atoms of the MoS2, in UHV molecules mainly chemisorb on MoS_2 surface defects, such as mirror twin boundaries (MTB) or sulfur vacancies.

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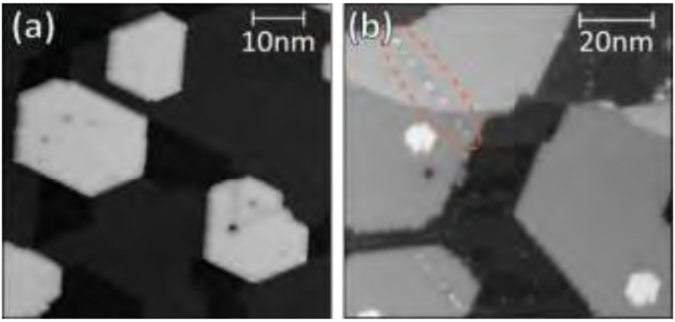

Iron oxide nanoparticles for t1 positive contrast in magnetic resonance imaging.

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Iron oxide nanoparticles (IONP) are well-known owing to their magnetic properties and their potential as Magnetic Resonance Imaging (MRI) probes. For several years, IONP-products were clinically available, but industry discontinued the production of these nanoparticles due of the lack of a clear application. The main reason for this is their typical signal in MRI, due to their superparamagnetic behavior, they provide the so-called "negative" contrast, a darkening of the tissue there where the IONP accumulate. For many diseases, this type of signal is far from optimal for diagnosis. [1-3]

To get the best of two worlds, i.e., the bright signal typical in Gd chelates plus the biocompatibility and multifunctional character of the IONPs, we're developing IONP that can provide positive contrast, a brightening of the tissue where the nanoparticles accumulate.

In this work we will present our most recent results showing different synthetic routes to produce IONPs for positive contrast in MRI and their application in the diagnosis of cardiovascular diseases.

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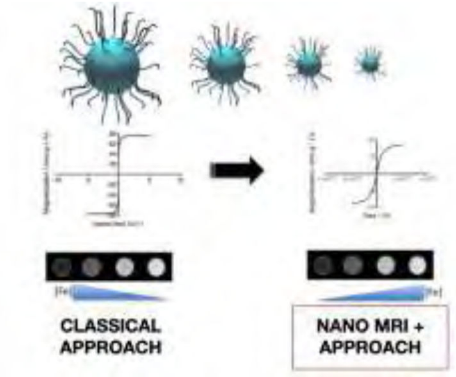

Figure 1: NanoMed+ project approach to MRI.

Bionanocomposites as sustainable materials for food packaging

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Biodegradable biopolymers are sustainable alternatives to conventional plastics for food packaging applications. To compete with synthetic polymers biopolymers needs to meet the requirements of cost-effective materials ensuring the mechanical and gas barrier characteristics of food packaging. Additionally, it is demanded to step towards active packaging, which means that packaging material need to interact with the food product to enhance its shelf life, contributing to reduce food waste. In this context, polysaccharides have been exploited to develop edible and biodegradable films due to their functional and sustainable characteristics and the integration of different fillers, such as clays, metal oxide particles and graphene derivatives, bring great challenges to the field of active food packaging [1].
The combination of the fillers, namely reduced graphene oxide (rGO), multiwalled carbon nanotubes (MWCNT), and zinc oxide, to design new formulations based on polysaccharides (starch, alginate and chitosan) allow to produce biomaterials with enhanced mechanical and barrier properties, conferring functional properties as antioxidant capacity, antimicrobial activity and/or electrical conductivity [2-5]. Electrical conductivity is a required property for the processing of food at low temperature using electric fields (Figure 1). Therefore, these bionanocomposites have a great potential as innovative and active food packaging.

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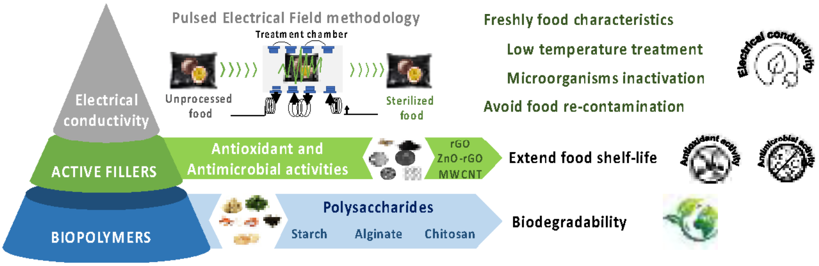

Figure 1: Electrical flexible bionanocomposite development.

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Silica-based glyconanoparticles for biomedical applications: from the inmune system to infection diseases

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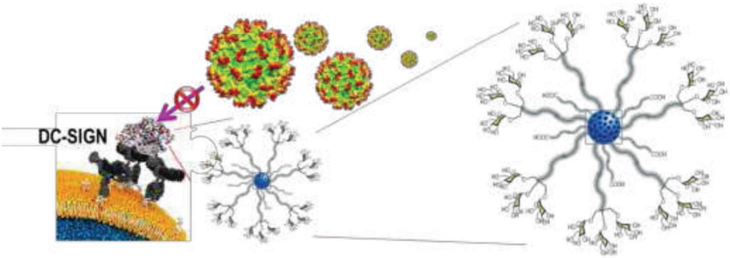
DC-SIGN (Dendritic Cell-Specific Intercellular adhesion molecule-3-Grabbing Non-integrin) is a C-type lectin presented on the surface of immature dendritic cells and plays a key role in the immune response and viral infections.[1] This lectin recognizes mainly fucosylated and mannosylated glycoconjugates. Our research group is interested in the study of this carbohydrate-protein interaction, both blocking and internalizing, of multivalent sugar-decorated glycoconjugates with this lectin due to the enormous relevance in many biological applications.[2]

In order to gain more insights, we proposed the use of silica-based nanoparticles as platforms for a multivalent carbohydrate presentation with biomedical applications. For this purpose, we focused on the design and preparation of different carbohydrates and their respective multivalent system based in glycodendrimers, as well as the conjugation to biocompatible silica nanoparticles. This silica-based nanoparticles could be act as virus inhibitors or modulator in adaptative immune response.



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PRODUCTION OF SILVER NANOPARTICLES USING BACTERIAL-CULTURE BROTHS OF THREE BACTERIAL ISOLATES, PHYSICO-CHEMICAL CHARACTERIZATION AND STUDY OF THEIR APPLICATIONS

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The use of biological methods for producing nanoparticles has some drawbacks but also some advantages in respect to other methods, among the last ones for instance the lack of use of toxic chemical compounds and the possibility of applying biological diversity to produce nanoparticles with different corona composition, thus producing materials with different properties.

The work we present was centered in the synthesis of silver nanoparticles (AgNPs) by using stationary-phase bacterial-culture broths from three bacterial isolates from the Tinto River: *Pseudomonas fulva, Ochrobactrum sp.* and *Lysinibacillus sphaericus*. Culture media used were either standard nutritive medium (containing NaCl) or medium without NaCl. Primary studies by our group showed that the presence or absence of NaCl affects the synthesis process [1].

For each synthesis using different bacteria broths kinetics were analyzed and physicochemical characteristics of the AgNPs produced determined.

For each type of AgNPs, essays were performed to estimate their possible applications as antibacterials, alone or in synergy with antibiotics, by determination of the Minimal Inhibitory and Minimal Bactericidal Concentrations (MIC and MBC), and Fractional Inhibitory Concentration Index (FICI) [2] for synergy with classic antibiotics as ampicillin, nalidixic acid and streptomycin.
Also, their properties as catalyzers for discoloration of the dyes carmin indigo and bromocresol green, in oxidative or reductive degradation reactions using $K_2S_2O_8$ or $NaBH_4$ respectively, were analyzed. The efficiency of the AgNPs for detecting metal ions in aqueous solutions was also tested in terms of Limits of Detection (LOD) and Limits of Quantification (LOQ) for Hg, Cu, Cd, Ni, Pb and Zn.

The results indicate that some differences exist in the kinetics of synthesis, and physicochemical properties of the nanomaterials obtained with the different bacteria. As well, all the nanoparticles were active against the six bacteria (three gramnegatives and three grampositives) used as test for antibacterial activity, but with different efficiencies, more effective against gramnegatives than grampositives and especially effective against *Pseudomonas aeruginosa*. Synergy was also observed for some of the AgNPs with some of the antibiotics tested with best results in the case of streptomycin. Also, some nanoparticles were able to aggregate or disaggregate in the presence of metal ions, and LOD and LOQ [3] were determined, showing a particular sensitivity of the nanoparticles to the presence of Pb or Cu and less to Ni or Zn. Finally, the presence of some of the nanoparticles facilitates the degradation of the tested dyes, been very pronounced for the case of bromocresol green when oxidized with $K_2S_2O_8$.

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Multiparametric Toxicity Assessment of Consumer-Relevant Nanomaterials in Intestinal Epithelial Caco-2 Cells

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The rapid progress in the development and application of nanomaterials (NM) in various areas such as industry, environment, agriculture, and biomedicine raised serious concerns regarding their safety to the human health and the environment [1]. The gastrointestinal tract is a likely route of entry for many NM, both by intentional ingestion or via nanoparticle (NP) dissolution from food containers or by secondary ingestion of inhaled particles [2].

In this study, our objective was to evaluate the influence of the chemical composition [Ag, Au, TiO_2, SiO_2 and graphene oxide (nano_GO)], primary size (10, 30 and 60 nm for AgNP and AuNP), crystal structure (rutile/anatase and anatase for TiO_2NP) and surface coating (citrate and PEG) for NM toxicity in a human intestinal barrier model. Caco-2 cells were exposed to various concentrations of NM (0.8-48 $\mu g/cm^2$) for 24 h and cytotoxicity was investigated by determining changes in cell morphology, cellular metabolic activity, plasma membrane integrity, intracellular levels of reactive oxygen species (ROS) and ATP. Changes in DNA integrity (strand breaks and oxidative damage) were also assessed.

No evident changes in Caco-2 cells morphology have been detected after exposure to any of the tested NM. However, large clusters of NM aggregates/agglomerates were visible, particularly at high concentrations. Our data showed a concentration-dependent reduction in the metabolic activity of Caco-2 cells exposed to the AgNP (AgNP_10 > AgNP_30 >AgNP_60) but no changes in plasma membrane integrity compared to control cells were observed. At the same time, citrate-coated AuNP also decreased cell metabolic activity of Caco-2 cells regardless of size, while PEG capping was effective in preventing changes in metabolic activity induced by AuNP_10. Regarding TiO_2NP, only the highest tested concentrations of rutile/anatase were able to induce a slight decreased in the metabolic activity of cells. Among the non-metallic NM, nano_GO proved to be more cytotoxic than SiO_2NP, inducing a greater decrease in cellular metabolic activity, 48% *vs* 19%, respectively. Only exposure to AgNP significantly increased intracellular ROS of Caco-2 cells to levels of 103% relative to the control, whereas all tested NM induced an increase in intracellular ATP levels. At the same time, only AgNP significantly increased DNA strand breaks.

Based on the obtained cytotoxicity profile, the tested NM can be ranked for cytotoxicity as AgNP > nano_GO > AuNP > TiO_2NP ~ SiO_2NP. The cytotoxic effects of the tested NM were more visible at higher concentrations and the smallest particles were the most cytotoxic. Additional research is needed to unravel the mechanisms of action and properties responsible for NM-mediated toxicity in human intestinal barrier models.

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Acknowledgments

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Phase controlled synthesis of 2D-MTe$_2$ (M=Mo, Ir) on epitaxial graphene

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Transition metal chalcogenides (TMCs) have been the subject of increasing interest for the condensed matter community in the past years. Among TMCs are those with a stoichiometry MTe$_2$, where M is a transition metal (groups IV-X), the so-called transition metal ditellurides (TMDTs) [1]. TMDTs show a very rich landscape of physical properties that depends not only on the transition metal but also on their thickness and crystallographic structure. For instance, the semiconducting hexagonal phase of MoTe$_2$ shows an indirect band gap in the bulk (2H phase) or a direct band gap at the monolayer (1H) [2] while its distorted octahedral phase (1T') is a three-dimensional topological Weyl semimetal predicted to exhibit quantum spin Hall (QSH) effect at the monolayer thickness [3]. Another example is the metastable 1T-IrTe$_2$ phase, which suffers structural phase transitions showing a competition between charge ordering and superconductivity that depends on its thickness [4]. Phase control has in fact emerged as an interesting approach to tune the properties of TMDTs [5].

Here, we report the growth of 2D islands of MoTe$_2$ and IrTe$_2$ via molecular beam epitaxy (MBE) on epitaxial graphene over Ir(111) (Fig. 1(a)). We demonstrate great control of the formation of their different structural phases (Fig. 1(c), 1(d) and 1(g)) by varying the substrate temperature (Fig. 1(b)) or tuning the Te:M ratio during growth (Fig. 1(e)). Their structural and electronic characteristics are studied by means of scanning tunneling microscopy (STM).

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Figures

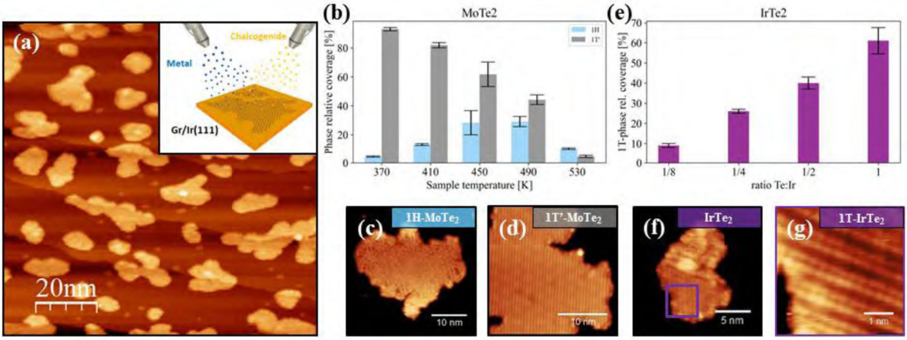

Figure 1: (a) Large STM image of IrTe$_2$ islands grown on gr/Ir(111) (V=-1V; I= 0.1nA). Inset shows a sketch of the growth procedure. **(b)** Barplot shows the relative coverage of 1T'- and 1H-MoTe$_2$ phases at different growth temperatures. STM images of **(c)** 1H-MoTe$_2$ (V=0.5V; I= 0.1nA) and **(d)** 1T'-MoTe$_2$ islands (V=1V; I= 0.1nA). **(e)** Barplot shows the relative coverage of 1T-IrTe$_2$ for different Te:Ir ratios. **(f)** STM image of an IrTe$_2$ island (V=-1V; I= 0.1nA). **(g)** Close-up showing 1T-IrTe$_2$ dimerization (V=-0.2V; I= 0.7nA).

Spin and Valley Filter Based on Two-Dimensional WSe_2 Heterostructures

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In this work we investigate the possibility of inducing and controlling spin and valley polarizations on different potential profiles of two-dimensional tungsten diselenide (WSe_2) heterostructures. We study the case of single and double-potential barrier configurations. We focus on the resonant regime and how this effect allows the spin and valley polarizations. Exchange valley splitting is provided by the magnetic proximity effect, with the advantages that the splitting is dictated by the exchange interaction strength and that no applied magnetic field is required. This allows a convenient scenario for obtaining the tuning processes. Moreover, due to the versatility of being either positive or negative valued, this description opens up the possibility of tuning the valley splitting sign and magnitude together.

Furthermore, we analyze the possibility of promoting valley and spin polarization inversions on transition metal dichalcogenides (TMDC) layers under the effects of time-dependent external potentials, such as time-oscillating gate voltages or laser irradiation. Different mechanisms are analyzed to synchronize the physical parameters of the proposed system, such as the Fermi energy, the frequency and amplitude of the time-dependent potential, and the external gate voltages, to optimize the time-dependent transport properties, such as the induced switching effects of the transport of the systems.

These results validate the proposal of double quantum well structures of WSe2 as candidates to provide spin- and valley-dependent transport within an optimal geometrical parameter regime [1].

This work was financed by FONDECYT- Chile, under Grants No. 1180914 and No. 1201876; FAPERJ-Brazil, under Grants No.E-26/202.567/2019; CNPq-Brazil, and the Instituto Nacional de Ciência e Tecnologia (INCT) em Nanomateriais de Carbono.

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Porphyrin functionalized silicon microdevices for photo-induced cell death

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Abstract

Photodynamic therapy is a promising cancer treatment strategy. A specific light source induces the excitation of photosensitizers which, under irradiation, are able to trigger the production of ROS that cause cell death. Porphyrins are one of the most promising photosensitizers, and their performance can improve through conjugation to delivery systems. We have studied the use of porphyrin-functionalized chips in photodynamic experiments with HeLa and Raw 264.7 cell lines.

The results have showed that porphyrin-functionalized chips retain their ability to be internalized by HeLa cells. Photoactivation induced a dose dependent cytotoxic effect in the presence of soluble porphyrin. Moreover, the internalization by HeLa cells of a number of functionalized chips can induce their death under irradiation conditions, while the internalization of non-functionalized chips does not produce observable cell alterations. A more marked effect and a higher microchips internalization ability was observed in the phagocytic Raw 264.7 cell line.

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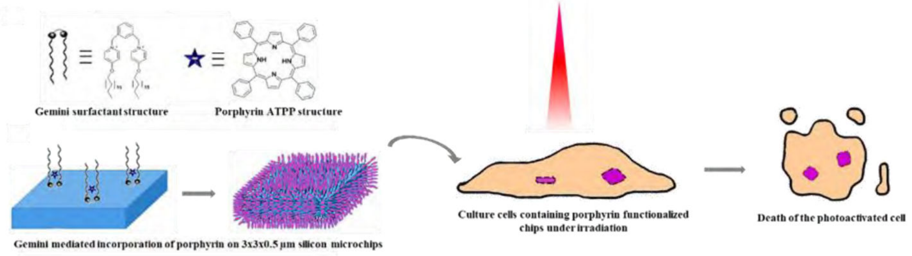

Figure 1: Scheme of the photoactivation experiments with porphyrin functionalized microchips in cultured cells.

Towards a wearable magnetometer

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Magnetoencephalography (MEG) is a technique for studying brain activity by measuring the magnetic fields induced by electrical currents generated in neurones. Currently, the devices that allow MEG have strong limitations such as their operation, size, ambient conditions and cost. The project pursues the development of an integrated magnetometer using the properties of diamond color centers, in particular, the negatively charged nitrogren-vacancy centers or NV centers [1][2][3][4]. They are especially interesting because of their unique properties for high resolution magnetometry. The spin of the electron that is enclosed within the defect can be manipulated at room temperature. Leveraging its properties, the goal is to develop a wearable magnetometer, that allows high spatial and time resolution and operates at room temperature.

The long-lived spin states and optically detected magnetic resonance allow a high sensitivity with nanometer scale spatial resolution.

We have demonstrated, using a diamond single crystal, manipulation of the electron spin, polarization and read out using a microwave antenna. The microwave field is used to manipulate the orientation of electron spins through the electron-spin resonance tuned by an external magnetic field. The electron spin is optically initialized using laser radiation and the photoluminescence spin-readout return from NV centers provides the information about the applied magnetic field.
As part of the roadmap to an integrated device, in the next steps we will miniaturise the device and investigate the way to fabricate the material using annealing and irradiation of a polycrystalline diamond wafer.

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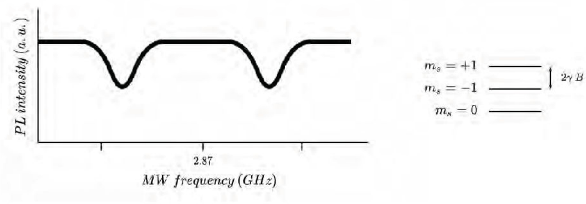

Figure 1: Due to the Zeeman effect, under an external magnetic field, the energy level splits resulting in the shifting of the PL in the optically detected magnetic resonance (ODMR) spectrum.

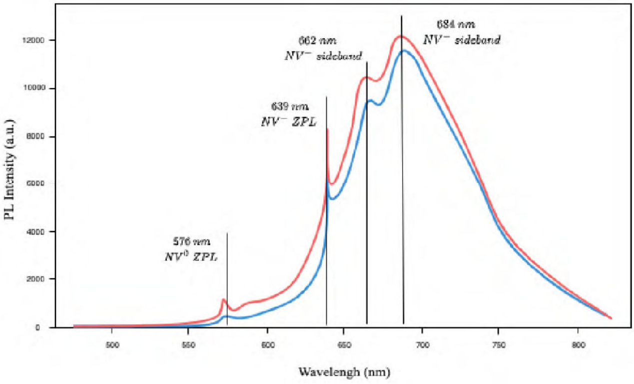

Figure 2: Photoluminescence spectra for an NV spin ensemble embedded in a single crystal diamond (red) and a polycrystalline diamond (blue). The typical luminescence curve representing the intensity as a function of the wavelength with the zero phonon lines (ZPL) and the phonon sidebands.

DNA Nanostructures for enhanced cellular uptake

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A remarkable strategy with increasing relevance in the desing of antitumoral therapies is based on the conjugation of anti-cancer drugs to molecules such as lipids or receptor ligands. [1] This results in the improvement of both their administration and their pharmacological properties. Following this approach, several studies have been performed to analyze oligonucleotide-molecule conjugates. [1,2]

In this work, a study regarding the properties of conjugates comprising an anti-metabolite nucleotide drug (floxuridine), with anti-tumoral activity, and a fatty acid has been performed. Therefore, the first step done was the incorporation of the desired fatty acid onto a solid support, allowing its use for the solid phase synthesis of the oligonucleotide conjugate.

Moreover, we studied the internalization effect of these molecules in tumoral cell lines sucha as HeLa and HCC2998. Finally, the cytotoxicity of these conjugates was assessed in the same cancer cell lines. Such conjugates are expected to show antiproliferative activity due to their metabolic activation by nuclease degradation, generating floxuridine mono-phosphate.

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Fluorescence enhancement with metasurfaces structures

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Metasurfaces have been already used for fabrication of flat and lightweight optical components, such as gratings, lenses, beam shapers (holographic phase masks, colour filters, and absorbers) [1]. Furthermore, these types of structures offer the possibility of tailoring the excitation and emission of fluorescent molecules by controlling the light propagation at nanoscale making them suitable candidates for biosensing applications [2].

Here we propose a low-cost metasurface platform consisting of metallic aggregates with random distributions for fluorescence enhancement comparable with results achieved by artificially engineered structures. We investigated the fluorescence emission of Rhodamine 6G (R6G) dispersed in polymethylmethacrylate (PMMA) or ethanol and coated on top of metallic nanoparticles. To better analyse the fluorescent enhancement, we studied three different concentrations of R6G (C1 = 50 µM, C2 = 10 µM and C3 = 5 µM), and three films thicknesses: 230, 190 and 170 nm. The analyzed metals are gold, aluminium and silver, and the substrates employed in this investigation are silicon and glass. The nanoparticles were obtained by e-beam evaporation of either discontinued layers (very thin- 2–4 nm-thick mass equivalent) or continuous layers nanostructured by thermal annealing [3]. Figure 1 show the variation of fluorescence intensity depending on fluorophore deposition characteristics. The best results concerning the fluorescent intensity were obtained when R6G was dispersed in PMMA, the role of PMMA being to protect the fluorophore luminescent properties from degradation when drying in normal atmosphere. Also, the presence of metasurface significantly increases the fluorescence emission. The results demonstrate that we can achieve an intensification of the fluorescence emission for R6G fluorophore up to 423 folds, depending on the geometry and distribution of the metallic nanostructures.

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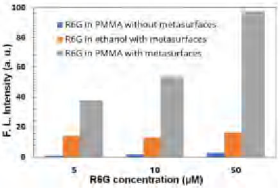

Figure 1: Variation of fluorescence intensity depending on fluorophore deposition characteristics (dispersed in Ethanol or PMMA) w/wo metasurface.

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Soft UV – Nanoimprint Lithography for Resonant Nanopillars fabrication

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Nanoimprint lithography (NIL) is a high resolution, low cost, high throughput lithography technique that has been at the forefront of technological advances in nanofabrication of the last couple of decades, especially due to its scalability features (from research to industrial level).
The use of resonant nanopillars (RNPs) arrays as optical biosensors has been extensively studied, thanks to their promising performances of biological detection with good sensitivity and limit of detection.
In this work we evaluate the use of NIL technique for the fabrication of RNPs arrays and describe the production in a step-by-step manner..

Figures

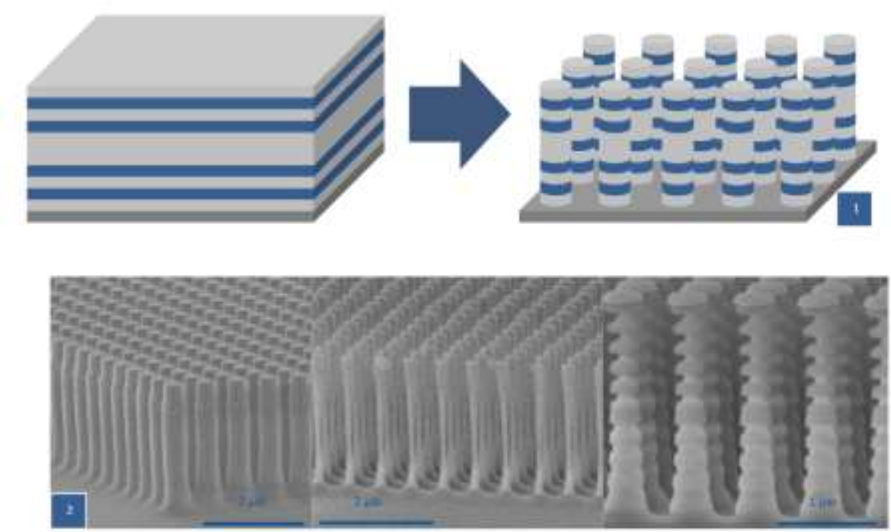

Figure 1: Figure 1. From bulk raw material to nanostructured surface. Figure 2. SEM images of different types of RNPs

Proton Transport through Peptides Nanotubes

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Peptide nanotubes consist of cyclic peptides piled on top of each other and held together by hydrogen bonds, making them similar to carbon nanotubes in morphology and aspect ratio. These materials are interesting both from the fundamental point of view and for the possible technological applications. They have been employed in biocompatible devices and as drug-delivery agents and are also promising proton conducting materials for the development of fuel cells, batteries, sensors and other advanced technologies. However, proton transport in peptide nanotubes is far from being well understood. Recent experiments on cyclic octa-peptides based on phenylalanine and functionalized with either lysine, arginine or histidine [1] showed an-order-of-magnitude-larger proton conductivity for the lysine-containing nanotubes. Theoretical simulations there included ascribed this to the different flexibilities of the side chains. However, what the role of the surrounding water molecules is on the proton transport through these systems had not been clarified. Inspired by these results, therefore, we carried out molecular dynamics simulations on these systems in aqueous environment to try gaining an insight into how water molecules can mediate the proton flow. For that, we considered various possibilities, considering both isolated nanotubes and bundles, which are known to be formed in the experimental self-assembled structures.

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Figures

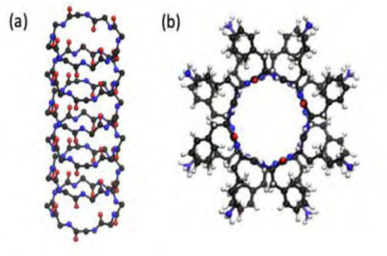

Figure 1: Side (a) and top views (b) of a section of the peptide nanotube c(KF)4; in (a) only the backbone is shown for clarity (*i.e.* the lysine (K) and phenylalanine (F) side chains are not shown). Each peptide ring contains 4 K and 4 F amino acids in an alternate fashion.

Numerical simularion of laser ablation processes in pulsed regime.

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Laser ablation processes of different metals has been the subject of research in the last decades, as they have various applications in some technological fields. In particular, they are used in monolithic interconnection of thin film photovoltaic modules. In this work we have simulated ablation processes in both nano and femtosecoseconds pulsed regime. Firstly, we have used the softawe COMSOL MULTIPHYSICS to solve the temperature evolution of a Copper piece irradiated by nanosecond pulses. Then, the molten phase was also modelled. This was already done by Chevallier et al. [1] for stainless steel, however, we have added multipulse regime with cooling phase as well as a temperature-dependent reflectivity.

Secondly, we have performed the same simulations by creating a (more computationally efficient) MATLAB code. Then, we have also used this language to simulate femtosecond regime. For doing that, the Two Temperature Model (TTM) [2] needed to be implemented. In this occasion, a silver piece was chosen for simulations. In both femto and nano second regime, a downward mesh velocity was defined to simulate the ablation process, considering the energy balance. The optical properties of the metals were obtained by using the Critical Point Model (CP) [3].

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Figures

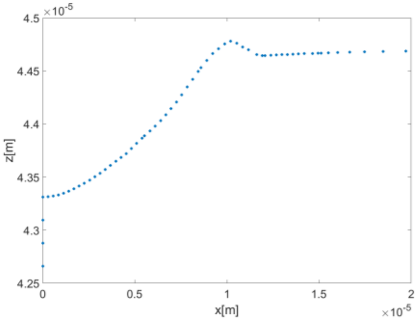

Figure 1: Ablation curve for copper piece, 12 ns laser, the molten phase was also modelled.

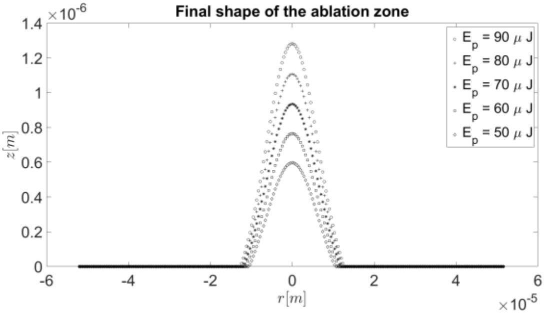

Figure 2: Ablation curves for silver piece, 350 fs laser, varying energy per pulse.

All-dry fabrication of WS_2 photodetectors on paper

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Given the high flexibility, biocompatibility, and biodegradability, paper-based devices are particularly suitable for the next generation of flexible electronics applications. However, fabricating electronic devices on paper remains a challenge due to the rough, fibrous, and permeable features of cellulose paper.[1] Up to now, inkjet printing of functional inks prepared by liquid-phase exfoliation of van der Waals (vdW) materials is probably the most common method, but the dispersion of the active material in the solvent and the removal of residual solvents are issues. The all-dry abrasion-induced deposition method based on the erosion of the vdW materials is a new promising approach to depositing vdW materials on paper substrate.[2]

As a typical class of vdW materials, transition metal dichalcogenides (TMDCs) such as WS_2 and MoS_2, are being used in various optoelectronic devices, which benefit from their remarkable electrical and optical properties.[3] Herein, we fabricated the high-performance WS_2 photodetection devices on the paper substrate by the all-dry abrasion deposition of the WS_2 thin film as the photoactive channel. We demonstrated that the frictional forces generated during the abrasion process are powerful to break the weaker vdW bonds between the layers, thus cleaving the WS_2 crystals to form the dense thin films. The high light-absorption efficiency of the WS_2 materials greatly enhances the photoresponsivity of optoelectronic devices. Importantly, the high surface roughness and porosity of cellulose fibers could provide a wider area of photoactivity for WS_2 photodetection devices compared to traditional flat substrates. The as-prepared WS_2 devices exhibit excellent photodetection performance over a broad wavelength range spanning from ultraviolet to near-infrared.

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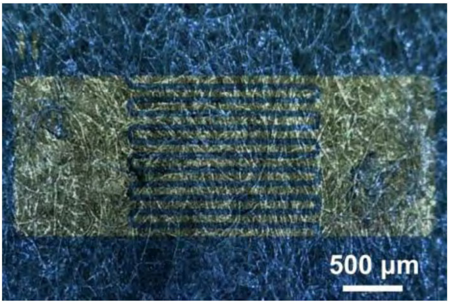

Figure 1: Optical micrograph of a WS_2 photodetector on paper.

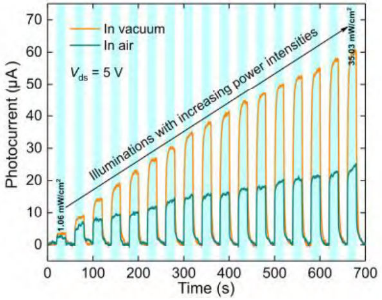

Figure 2: Photoresponse performance of the WS_2 device.

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