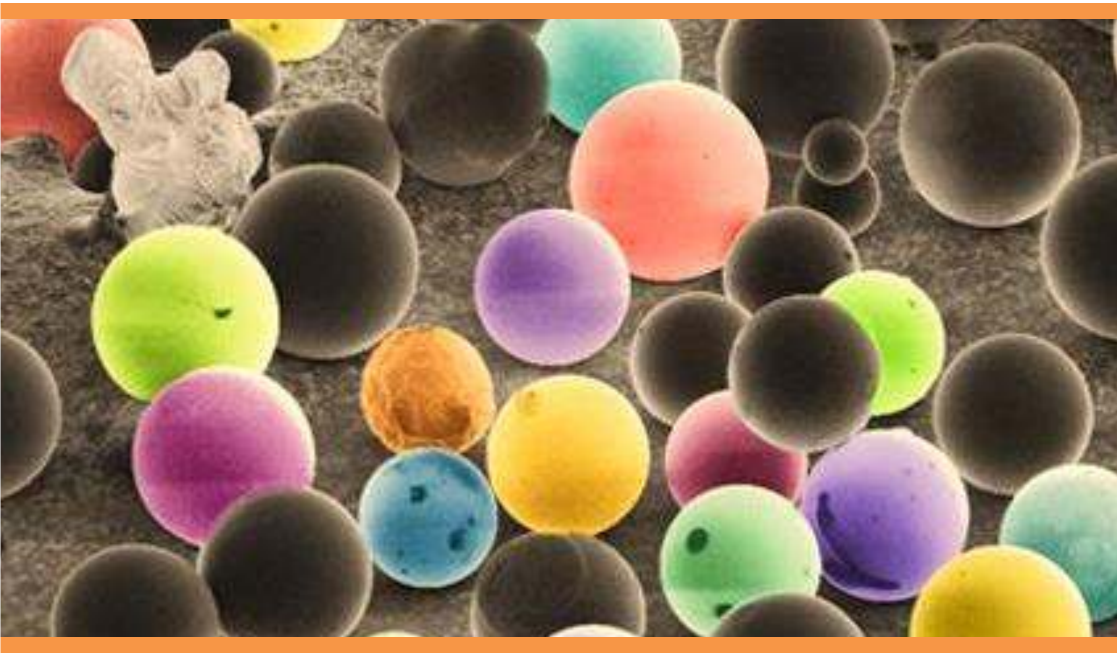
NanoSpainConf 2017

March 07-10, 2017 – San Sebastian (Spain)

ABSTRACTS BOOK



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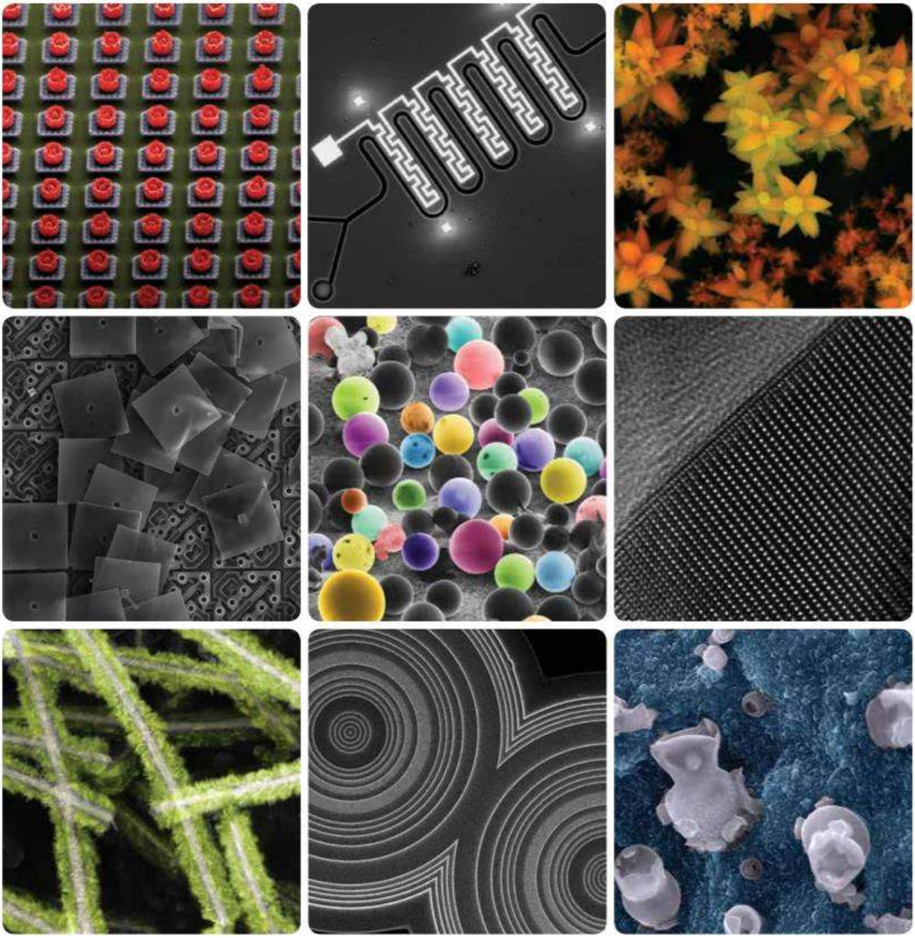

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NanoSpain Conf 2017

March 07-10, 2017 – San Sebastian (Spain)

Consolidated as a reference meeting of Nanoscience and Nanotechnology (N&N) in Spain, the NanoSpain2017 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.

Since 2004, year the event was launched, NanoSpain conference series is now an established and well-known meeting in Spain, aiming to agglutinate and coordinate the efforts made in the field of the Nanotechnology by Spanish groups from universities, research institutes and companies.

NanoSpain events facilitate the dissemination of knowledge and promote interdisciplinary discussions not only in Spain but among the different groups from Southern Europe.

Over the past years, NanoSpain conference became more and more multidisciplinary and 2017 won't be an exception. NanoSpain2017 will cover a broad range of current research in Nanoscience and Nanotechnology.

NanoSpain2017 will offer a multitude of renowned international Keynote and Invited speakers, contributed talks, posters and a commercial exhibition. In addition thematic parallel sessions will also be organised to enhance information flow between participants and in particular:

- Exchange information of current work in specific research areas
- Solve particular technological problems
- Look for areas of common ground between different technologies
- Provide contributions to specific reports

The following Thematic Parallel Sessions will be organised:

1. Nanobiotechnology
2. Nanotoxicology

We would like to thank all participants, speakers, sponsors and exhibitors that joined us this year.

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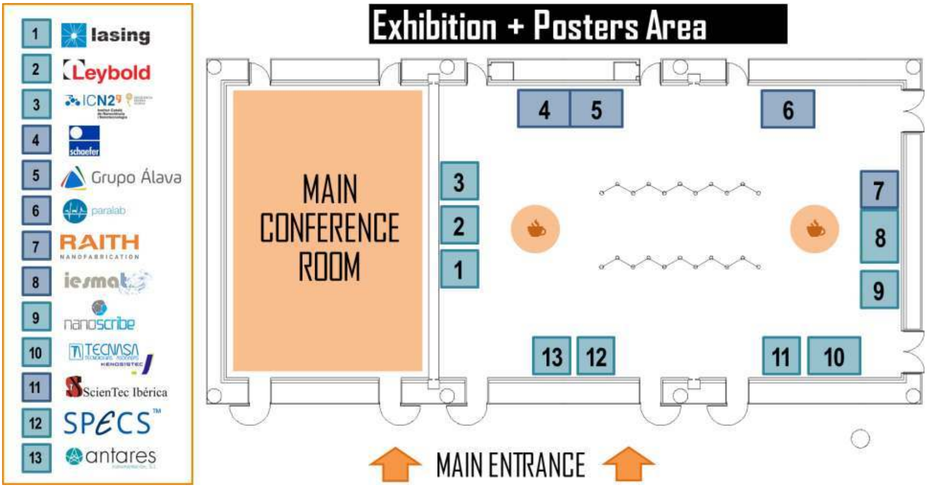

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Plenary, Keynotes and Invited Speakers

Driving Nanophotonics to the Atomic Scale

Javier Aizpurua

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Plasmonic nanocavities formed at the junction of two metallic interfaces provide a great platform to explore atomic-scale morphologies and complex photochemical processes by optically monitoring the excitation of their intense surface plasmonic modes. In recent years, optical spectroscopy of these cavities has proven to be extremely sensitive to atomic-scale features that determine the chemistry and the optoelectronics in the gaps. In this regime, classical theories fail to address the fine details of the optical response, and more sophisticated quantum theories are needed [1].

We develop a quantum atomistic description of the total energy and the optical response of metallic nanojunctions within Time-dependent Density Functional Theory (TDDFT) that allows to properly address atomic-scale features of the field enhancement and localization of light at the gap [2] (see Figure below), providing new keys to understand the ultraresolution obtained in molecular vibrational spectroscopy [3]. The small effective volumes associated to these new type of optical 'pico-cavities' are of particular interest in quantum nanooptics, as they provide large values of the coupling strength between the photons in the cavity and excitons of an emitter or mechanical vibrations of a molecule. We exploit this opportunity of large coupling in molecular optomechanics of single molecules [4,5].

The atomic scale is a challenging regime in plasmonics, progressively achieved experimentally. New theoretical tools, as those pointed out here, become necessary to understand this regime, and implement new concepts in optoelectronics, quantum nanooptics, and field-enhanced spectroscopy.

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Figure

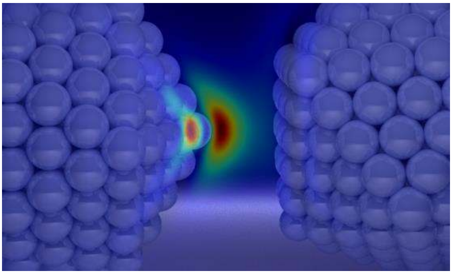

Figure 1: Time-Dependent Density Functional Theory (TDDFT) calculation of the electromagnetic field localized around atomic-scale features [2] in a metallic 'pico-cavity' to be exploited in molecular spectroscopy, nanoscale optomechanics, and optoelectronic transport. The blue spheres represent sodium atoms building the plasmonic cavity. Bright colours from red to blue express the intensity of the electromagnetic field. (in collaboration with D. Sánchez-Portal's group).

Triggering reactions on metal surfaces with femtosecond laser pulses

Maite Alducin

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Femtosecond laser pulses have proven to be very efficient in promoting reactions at metal surfaces that cannot be initiated by thermal activation [1,2]. The wavelength and intensity of the laser pulse determine if a reaction starts as a direct excitation of the adsorbate or, on the contrary, if it is an indirect mechanism in which the substrate efficiently absorbs the laser energy to subsequently release it on the adsorbates. The latter is precisely the mechanism that better accounts for reactions induced by UV/vis lasers on metal surfaces. In this talk I will focus on such kind of photodesorption processes and present recent results on the desorption of molecular O_2 from Ag(110) [3] as well as on the recombinative desorption of H_2, D_2 and HD from Ru(0001) [4]. These two systems will allow us to extract information on how the desorption yields and dynamics are affected by the chemisorption properties and by the presence of additional adsorbates. In this respect, our newly developed *ab initio molecular dynamics with electronic friction* (AIMDEF) [5,6] method, which is based on the *local density approximation* (LDFA) [7] and recently extended to account for the hot electrons created by the laser pulse trough a time-dependent electronic temperature [4], constitutes a powerful tool to get insight in the nanoscale dynamics of the reaction.

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Figures

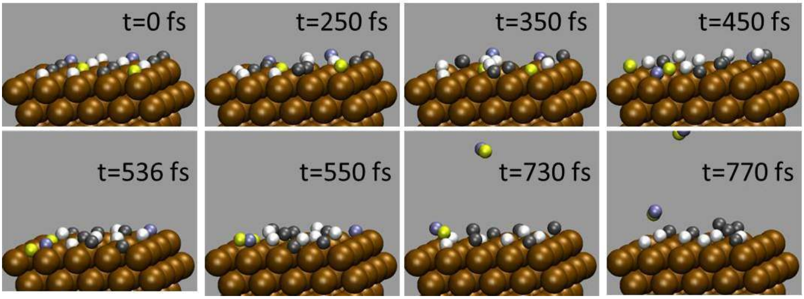

Figure 1: Snapshots of one of the AIMDEF simulations for an equal (8:8) H:D isotope mixture on Ru(0001) that ends with two HD desorbing molecules. White and black spheres are respectively the non-desorbing H and D atoms, yellow and blue spheres are the desorbing H and D atoms, and golden spheres are Ru atoms

Thermo- and magneto-electric Effects in Superconducting Nanostructures

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The main focus of this talk is on superconductors with a spin-split density of states due to, either an external field, or the proximity of a magnetic insulator. The interplay between the superconducting state and spin-splitting fields leads to striking transport phenomena [1] and devices that are discussed in this talk.

These include:

(i) a thermoelectric transistor based on ferromagnetic insulator- superconductor bilayers [1] ,
(ii) the occurrence of a thermophase in S-FI-S structures [2],
(iii) the possibility of using FI-S in high sensitive detectors and thermometers[3], and
(iv) a heat valve based on a ferromagnetic Josephson junction [4].

In addition I will also discuss first experiments in this field that basically shows the feasibility of such devices[5].

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Figures

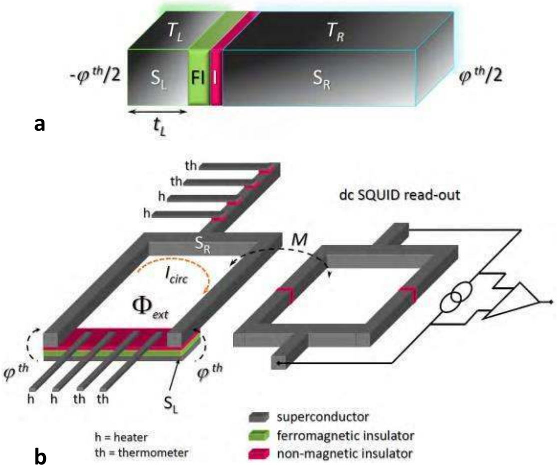

Figure 1: a) Josephson junction between two superconductors and a ferromagnetic insulating layer. b) Setup for measuring the tehrmophase induced by the temperature difference between the superconducting arms on the left loop. The generated supercurrent can be measured with the help of a second SQUID (right loop).

Nanostructured coatings: from lab to application

Marta Brizuela[a], Cecilia Agustín[a], José Luis Viviente[a], Iñigo Braceras[a], Pablo Corengia[a], Teresa Cristina Rojas[b], Juan Carlos Sánchez-López[b]

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Different nanostructured coatings have been explored by the authors: from solid lubricant coatings, protective coatings and finally anti-reflective coatings.

MoS_x-WC nanostructured coatings have been studied by the authors as a solid lubricant coating to be used in different mechanisms as ball bearings, harmonic drive® gears, etc. These coatings were synteshized by magnetron sputtering and tested under different tribological conditions (different levels of humidity, vacuum and even space). Their structure was a multilayer coating of nanoperiod. Their tribological properties over-performed the pure MoS_x coatings that are the state-of-the art solid lubricant used in space. Finally these coatings were tested in a real component as an harmonic drive® gear showing a great benefit [1].

Multilayered CrAl(Y)N coatings of nanoperiod were deposited on M2 and 316 steel substrates and heated to 1000 °C in air for 2 h to study their oxidation mechanism and thermal stability. The reactive element effect of Y is confirmed but differs from the typical observed in alloys. The ion interdiffusion of substrate element plays an important role in the oxidation process. The Y presence retards the iron outward diffusion by forming oxides in M2 and yttrium nitride in 316 steels. The microstructural analysis determined that yttrium migrates to the grains and interface of the oxide scale and to the nitride column boundaries. These coatings can be of interest in applications as supercritic steam turbine components [2]

SiO_2 nanostructured Coatings have been synthesized and integrated in a graded-refractive-index multilayer system deposited onto solar glass in order to provide antireflection properties. The coatings are synthesized by sol-gel and evaporation-induced self-assembly (EISA) method and deposited by dip-coating. This technique has permitted to obtain mesostructured porosity and a high control of the void fraction in the coating [3]. Environmental ellipsometric porosimetry (EEP) has proved to be a useful technique to determine porosity (Bruggeman effective medium approximation) and refractive index change with humidity. These measurements provide water adsorption-desorption isotherms thus permitting the calculation of pore size distribution of the coatings [4].

Optical properties (transmittance and reflectance) and mechanical properties (nanohardness, adherence) have been also crucial to select coatings for designing a durable, broadband, scratch resistant, AR system for cover materials in HCPV applications.

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Novel theories for the thermoelectric effect

Roberto D'Agosta

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Understanding of the thermoelectric effect poses critical challenges for the theorists, since it entails a comprehensive description of both electron and thermal transport, phenomena usually associated with diverse mechanisms, and more importantly with different energy scales. In the last few years, tremendous progress has been made in building models to describe these transport effects, starting from either the Boltzmann equation or the Landauer formalism [1]. In this talk, I will present some of the theoretical advancements made by the Spanish consortium nanoTherm [2], comparing them with the actual international outlook, and in some case bridging the gap with experiments. An overlook of the experimental progress is presented in the talk of Dr. O. Caballero and Dr. M. Martinez.

I will focus my attention to two of the most recent developments, namely an effective description of phonon thermal transport [3] that is able to describe the confinement effect in nanowires of decreasing diameter, and a theory for the Seebeck coefficient where we take into account the effect of the electron exchange and correlation energy [4].

Finally, I will take the opportunity to introduce a novel "Red Tematica" on the thermoelectric theory.

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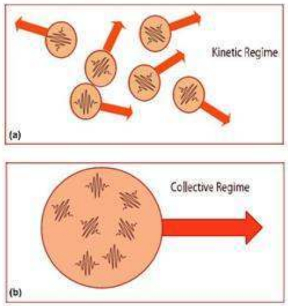

Figure 1: Different energy and time scales define the regime for thermal transport. From [4].

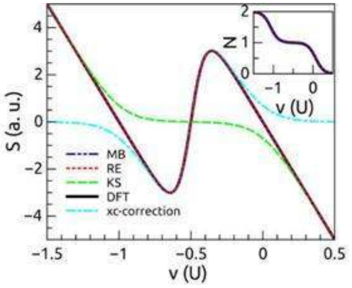

Figure 2: The exact Seebeck coefficient (black and red lines) for a strongly correlated electron system might differ significantly from the prediction of standard ab-initio methods (green lines). From [4].

Multisectorial applications of graphene

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Tecnalia approaches the identification and development of potential innovative graphene applications from a societal point of view, by identifying current needs in a wide-range of fields, such as energy, health, industry, construction, etc. Our sound technological knowledge enables us to identify problems and applications for this new nanomaterial, which can greatly benefit society. Once identified, thanks to our state-of-the-art laboratories, we are able to develop prototypes (both at lab and pilot scale) with an aim to solve the identified problems. Finally, a feasible solution is designed and transferred to industry.

TECNALIA has several on-going developments of graphene-derived products, such as:

- Electrodes for batteries & supercapacitors for energy storage
- High thermal dissipation composites (e.g. for aerospace and electronics applications)
- Thermal interface materials (e.g. for electronics applications)
- Light-weight composites (e.g. for transport applications)
- Electrodes for water desalination
- Conductive inks for printed electronics
- Conductive coatings as novel electrodes
- Membranes for separation processes (e.g. for chemical industry applications)

The following two examples will be presented in detail: (1) Electrodes for batteries [1] and (2) high thermal dissipation composites for aerospace applications [2].

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Figures

Figure 1: Cathodes for Li-S batteries

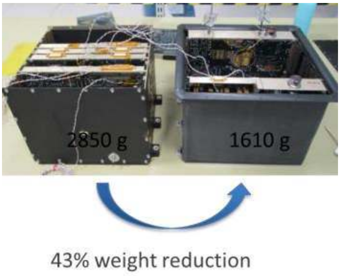

Figure 2: Light-weight composites for aerospace applications

Tracking nanomedicines *in vivo* using PET imaging

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Imaging methods that report on drug biodistribution and pharmacokinetics in vivo should allow us to identify, monitor and improve the efficacy of novel therapeutic approaches based on nanomedicines. In order to support clinical trials and applications in these areas there is a need to develop simple radiolabelling methods for non-invasive imaging techniques to monitor their biodistribution and answer questions such as: How much nanomedicine drug is/stays in the target? Does it migrate to potentially sensitive organs? How is it cleared?.

Positron emission tomography (PET) is particularly well suited to answer these questions. It is the only clinically available non-invasive imaging technique that allows quantitative analysis of imaging signals with exquisite sensitivity (signal/background ratios) and adequate spatial/temporal resolution at the whole-body level. Taking examples from my own research group [1-10] and other researchers in the field, in this talk I will describe examples on how different PET radiolabelling methods have been used to track nanomedicines in preclinical and clinical studies.

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Moving forward with magnetic hyperthermia: can we profit from intracellular clustering of the magnetic nanoparticles?

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The possibility of using Magnetic hyperthermia (MHT) as a standalone therapy requires reaching acceptable therapeutic effects with minimum concentration of heating agent. With obvious advantages for the treatment of deep, inaccessible human tumors, MHT aims to increase the local tumor temperature up to apoptotic levels, with minimal side effects on the surrounding healthy tissue.[1] A necessary step to this aim is the design of field-efficient magnetic nanoparticles (MNPs) as heating agents within the intracellular environment. By numerical simulation of the response under magnetic fields, the magnetic parameters of MNPs such as magnetic anisotropy and dipolar interactions are optimized within a numerical model of the relaxation mechanisms so that the heating efficiency is preserved in the intracellular environment. The output of this protocol is the largest in vitro specific power absorption (SPA) values reported so far.[2] However, the role of dipolar interactions due to intracellular agglomeration found from the numerical solutions to be the main cause of changes in the magnetic relaxation dynamics of MNPs, is not yet completely understood. The experimental and theoretical body of data needs to be completed in order to unveil these mechanisms, especially for *in vitro* and *in vivo* conditions, before aiming a physical design of MNPs that can retain their heating efficiency in clinical hyperthermia experiments.

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Infrared nanoimaging and nanospectroscopy

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With the development of scattering-type scanning near-field optical microscopy (s-SNOM) [1], the analytical power of visible, infrared and THz imaging has been brought to the nanometer scale. The spatial resolution of about 10 - 20 nm opens a new era for modern nano-analytical applications such as chemical identification, free-carrier profiling and plasmonic vector near-field mapping.

s-SNOM is based on elastic light scattering from atomic force microscope tips. Acting as an optical antenna, the tips convert the illuminating light into strongly concentrated near fields at the tip apex (nanofocus) (Figure 1), which provides a means for localized excitation of molecule vibrations, plasmons or phonons in the sample surface. Recording the tip-scattered light as a function of sample position subsequently yields nanoscale resolved optical images, beating the diffraction limit in the infrared spectral range by more than two orders of magnitude.

Using broadband IR illumination and Fourier-transform spectroscopy of the tip-scattered light [2,3], IR spectra with 20 nm spatial resolution can be acquired (nano-FTIR). Near-field images and near-field absorption spectra of molecular vibrations in mid-infrared fingerprint region allow for chemical mapping, identification of polymer [3] and protein [4] nanostructures, and for quantitative measurement of the complex-valued local dielectric function [5]. Latest technical developments enable hyperspectral infrared nanoimaging and application of multivariate spectral data analysis.

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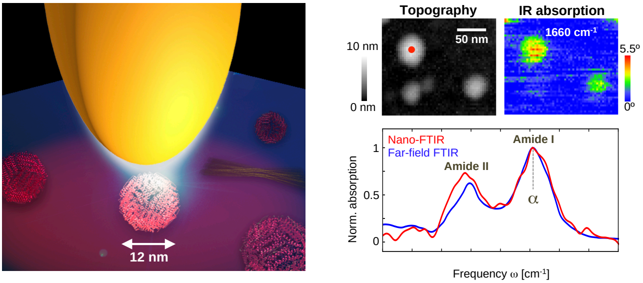

Figure 1: Infrared nanoimaging of a single protein complex (ferritin, 5000 C=O bonds, 1 attogram mass). Left: Illustration of the infrared illuminated tip of a near-field microscope on top of a ferritin complex. Right: Topography and infrared absorption image of three nanoparticles reveals that only two of them are protein complexes. The nano-FTIR spectrum (red) was taken on the complex marked by the red dot in the topography image.

Small is different: emergent paradigms and atomically precise nano structures

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Finite materials systems of reduced sizes exhibit specific forms of aggregation, phases, structures and morphologies, quantized electronic shell structures, dimensionality cross-over, and size-dependent evolutionary patterns, which are manifested in unique, nonscalable, size-dependent physical and chemical properties. Indeed, when the dimensions of materials structures are reduced to the nanoscale, emergent phenomena often occurs, that are not commonly expected, or deduced, from knowledge gained at larger sizes. Discovery, characterization, understanding and possible utilization of such emergent behavior of materials in the nanoscale are among the major challenges of modern materials science. Progress in theses directions is greatly facilitated, or even predicated, by synthesis, fabrication, separation and measurements of atomically precise nanostructures, and by theoretical investigations of their unique structural, chemical and physical properties. Computer-based quantum computations, simulations and emulations, are tools of discovery which enable uncovering emergent behavior in the nanoscale [1]. In this talk we employ such simulations, often in conjunction with laboratory experiments, in explorations of several atomically precise nanostructures, to address some of the basic origins that underlie the unique behavior of size-selected materials in the nanoscale, and highlight computational microscopy investigations of nanoscale phenomena in diverse systems. These include: (i) Nanocatalysis by size-selected cluster catalysts of nanometer dimensions [2a] and reassessment of the specific activity and size sensitivity of heterogeneously catalyzed reactions, e.g. ethelene hydrogenation catalyzed by nano-size platinum clusters supported on magnesia or amorphous silica surfaces [2b]; (ii) Monolayer- protected metal nanoclusters [3] and their self-assembled superlattices [3b], exhibiting stabilities and properties originating from superatom electronic shell-closing, atom packing, and interactions between protecting ligands ; (iii) The electronic structure and electrical transport characteristics – manifesting Fabry-Pérot interference patterns, described with tight-bonding and a Dirac relativistic formulation with position-dependent mass terms – of graphene nanoribbons, GNRs, with atomically precise widths and edges, including segmented GNRs (characterized by width-dependent energy band-gaps) comprised of junctions between nanoribbons of varying width [4]; (vi) Symmetry-breaking and formation of highly-correlated Wigner molecules [5a] in electron quantum dots [5a] and ultracold fermionic atoms, e.g. a few 10^{-9}K ^{6}Li atoms in laser-generated double-well confinements [5b,5c], exhibiting antiferromagnetic ground states modeled with exact numerical solutions of the microscopic Hamiltonian and mapped onto Heisenberg spin-chain and cluster Hamiltonians, as well as the t-J model [5c], suggesting the employment of finite ultracold atom systems in fundamental studies of quantum magnetism and high-T_c superconductivity.

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High Yield Seeded-Growth of Anisotropic Gold Nanoparticles

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Although recent progress of seeded-growth has made available an extensive library of anisotropic metal nanoparticles [1], the chemical complexity of the growth solution, often involving organic additives [2], and the structural instability of the seeds hinder the quest for high quality products. For the sake of synthetic simplicity, merging different synthetic protocols by finding common growth routes, is a mandatory step to reach a universal growth mechanism and reproducible fabrication. We show here that thermal treatment of small seeds results in extensive twinning and a subsequent drastic yield improvement (>85%) in the formation of pentatwinned nanoparticles, with pre-selected morphology (nanorods, bipyramids and decahedra) and aspect ratio [3]. The “quality” of the seeds thus defines the yield of the obtained nanoparticles, which in the case of nanorods avoids the need for additives such as Ag^+ ions. This modified seeded growth method also improves reproducibility, as the seeds can be stored for extended periods of time without compromising the quality of the final nanoparticles. Additionally, minor modification of the seeds with Pd allows their localization within the final particles, which opens new avenues toward mechanistic studies. All together, these results represent a paradigm shift in anisotropic gold nanoparticle synthesis.

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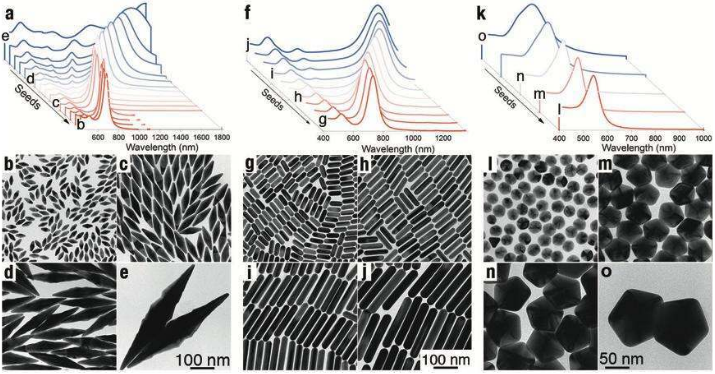

Figure 1: Universal character of thermally-treated seeds. Effect of seed concentration on the growth of bipyramids (a-e), nanorods (f-j) and decahedra (k,o). (a,f,k) UV-Vis-NIR spectra of colloids prepared with different seed concentrations and representative TEM images of nanoparticles prepared in a single growth step from different amounts of seeds.

Radiolabelling and *in vivo* imaging to assess regional drug distribution after lung administration

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Nanoparticles (NPs) have been under extensive investigation because of their high potential as nanocarriers (NCs) for a broad range of chemical entities, including drugs and chemotherapeutic agents. Most of the studies reported so far rely on intravenous administration. However, lung administration has recently gained attention, especially when the lung is the target organ, e.g. to treat lung cancer or airway diseases such as asthma, cystic fibrosis and chronic obstructive pulmonary disease [1]. Pulmonary administration offers numerous advantages as a delivery route compared to oral or intravenous administration, as it can prevent rapid metabolism while decreasing unwanted off-target side effects. However, pulmonary administration poses several challenges, especially in the pre-clinical setting. Regional distribution of the nanomedicine, residence time in the lungs and translocation to remote organs are essential parameters to predict therapeutic efficacy and to define the most appropriate administration pattern.

In this talk, different alternatives for the pulmonary administration of aerosolized nanomedicines in rodents will be discussed. The application of nuclear imaging techniques (Figure 1) to the assessment of the fraction of the aerosol deposited in the lungs, the regional lung distribution, the residence time in the lungs, drug release rate and clearance to remote organs will be discussed.

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Figures

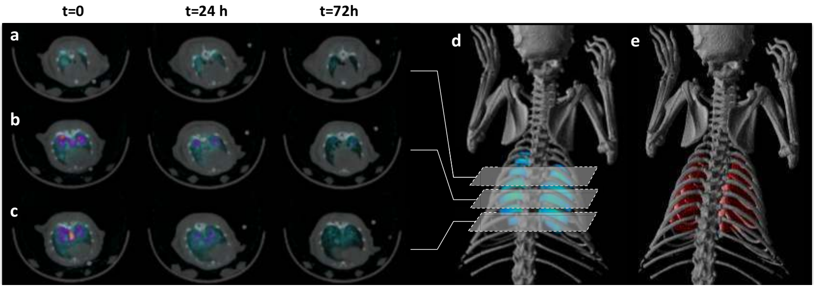

Figure 1: Example of Positron Emission Tomography (PET) images obtained at different times after lung administration of labelled nanoparticles in rats; (a-c) selected coronal slices from images obtained at different time points after administration. PET images are co-registered with Computerised Tomography (CT, grey scale) for appropriate localization of the radioactive signal; (d) volume 3D-rendered image showing distribution of the radioactive signal; (e) surface 3D-rendered image corresponding to the segmented lungs.

Designing biomolecular scaffolds for hybrid functional materials and nano-sensors

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Self-assembly of biological molecules into defined functional structures has a tremendous potential in nanopatterning, and the design of novel biomaterials and functional devices. Molecular self-assembly is a process by which complex three-dimensional structures with specified functions are constructed from simple molecular building blocks. We present the supramolecular assembly of modular repeat proteins, in particular designed consensus tetratricopeptide repeats (CTPRs), and their application as building blocks for the generation of functional nanostructures and biomaterials. CTPR proteins can be assembled into self-standing thin films,[1] monolayers,[2] and thin nanometer fibers.[3] In this work, we show the use of CTPRs as scaffolds to template: (1) Photoactive organic molecules.[4] In particular, CTPR proteins are used to organize organic chromophores, while preserving their structure. The unique self assembly properties of CTPRs have been exploited to generate ordered photoconductive films of the protein-porphyrin conjugates. (2) Gold Nanoparticles.[2] CTPR are used to template gold nanoparticles into ordered monolayers, and into structured thin films providing conductivity properties to the materials. (3) Fluorescent nanoclusters.[5] We show the ability of CTPR proteins to stabilize fluorescent gold nanoclusters. Since the structural and functional integrity of the protein template is critical for applications, protocols that retain the protein structure and function have been developed. A CTPR module with specific binding capabilities has been successfully used to stabilize nanoclusters and tested as a sensor.

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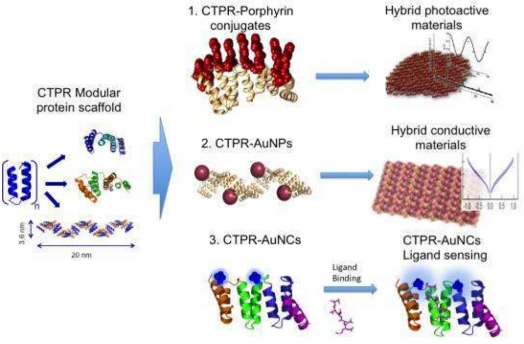

Figure 1: Shematic representation of hybrid protein based materials and nanostructures

Tunable optical properties of nanoporous anodic alumina structures by pulse anodisation

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Structurally engineered nanoporous materials attract plenty of attention due to their potential applications in areas such as electronics, photonics, drug delivery, energy, and so on. Nanoporous anodic alumina (NAA) produced by electrochemical etching of aluminum has become a popular material as a result of its cost-competitive fabrication processes and its outstanding set of properties such as self-organised nanoporous structure, straight cylindrical nanopores of high aspect ratio, optical properties, chemical and thermal stability [1].

Recently, different anodization approaches have been proposed to create new structures and pore geometries (e.g. pore diameter, interpore distance, porosity). They allow to tune the optical properties of NAA (e.g. photoluminescence, reflectance, absorbance, emission, etc.) and propose applications in optical biosensing and photovoltaic fields [2,3,4].

Distributed Bragg reflectors (DBR) are optical structures formed by the periodic repetition of two layers in depth with different refractive index and thickness and produced in NAA by stepwise pulse anodisation approaches (Figure 1). Other interesting optical structures are named gradient-index filters (GIF) in which the effective refractive index is continuously modified in depth in a sinusoidal or pseudosinusoidal way o profile. These structures can also be obtained in NAA by applying a sinusoidal current anodization and leads to an enhanced reflection of light in narrow regions of the UV-Visible-NIR spectrum.

In this work, we present a detailed study on the structural and optical characteristics of NAA-DBR and NAA-GIF structures and how we can tune the optical signal by modulating fabrication parameters.

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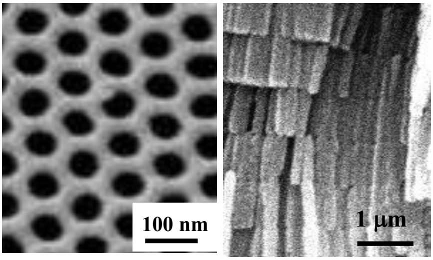

Figure 1: Top view (left) and transversal view (right) of a NAA structure formed by the periodic repetition of two layers with different refractive index and thickness (SEM image).

Atomic manipulation and morphology engineering in two-dimensional materials: from buckled Xenes to anisotropic MoS_2

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Making adjustable two-dimenasional (2D) materials is an emerging route to reach a superior control of new functional properties at the 2D level. Consideration will be given here to two distinct cases in this respect. On one hand is the case of the epitaxial Xenes, an emerging class of 2D monoelemental lattice; on the other hand is the artificial synthesis of MoS_2 nanosheets with an anisotropic fashion. By close analogy with graphene, epitaxial Xenes are comprised of monoelemental atoms arranged in a honeycomb lattice; unlike graphene, Xenes are epitaxially grown on substrates and exhibit a varying degrees of buckling and/or puckering in the lattice structure.[1] Examples in this respect are silicene, germanene, stanene, borophene, epitaxial phosphorene. Buckling in Xenes can be taken as a leverage to tune the electronic and quantum properties (see the pictorial sketch of a buckled Xenes with topologically protected edge states in Figure 1). Indeed, the electronic state of epitaxial Xenes can range from topological insulators to trivial insulators, semiconductors, and semimetals, depending on the configurational details (e.g. buckling, substrate, chemical functionalization, and strain); and topological transitions among these electronic states can be tuned by means of a buckling dependent elecrical field applied to the Xenes. An overview of the state-of-the-art on the epitaxial Xenes and of their potential in nanoelectronics will be here given.

A second case of anisotropy is based on the chemical vaour deposition of MoS_2 nanosheets on one-directional substrates. The highly conformal character of the growth allows for the achievement of an anisotropically modulated MoS_2 nanosheet (see the sketch and the related TEM image in Figure 2) where the phonon and electronic properties are observed to be strongly morphology dependent. The so-induced anisotropy in the MoS_2 nanosheet (that are isotropic in chatacter) results in a light polarization dependent Raman spectrum and periodic charge fluctuations.[2] Implications on the band-gap and strain engineering will be discussed.

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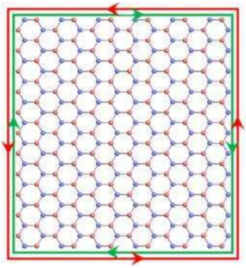

Figure 1: Pictorial sketch of an epitaxial Xene lattice with topologically protected edges states.

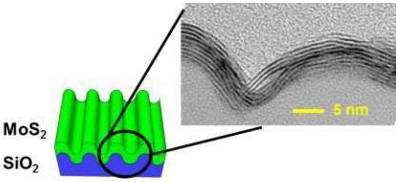

Figure 2: Sketch of an anisotropic MoS_2 nanosheet and corresponding TEM image

2D nanoscale electronics and optoelectronics

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The materials that have enabled the information technology revolution over the past decades will soon reach their physical limits. Novel nanomaterials and technologies have therefore become a major focus of current solid-state device research, with two-dimensional (2D) atomic crystals being one of the most promising candidates. Graphene, a 2D structure of carbon atoms with unorthodox electronic properties, is the most prominent representative of the 2D material family. More recently, transition metal dichalcogenides (TMDs) have come into the focus of interest, as these offer properties that complement those of graphene. Some TMDs are semiconductors with a sizable bandgap, which allows the construction of logic transistors, light emitters, photovoltaic solar cells, and other devices. In the first part of this talk, I will present some of our results on the development of electronic circuits based on 2D materials. Large-area MoS_2 growth by chemical vapor deposition, together with the development of 2D logic stages, enabled us to realize for the first time large-scale digital circuits, such as simple microprocessors. I will then review our activities on photovoltaic energy conversion, photon detection and electrically driven light emission in TMDs. In particular, monolayer p-n junctions, formed by electrostatic doping of WSe_2, and MoS_2/WSe_2 van der Waals heterojunctions will be presented. Upon optical illumination, conversion of light into electrical energy occurs in both types of devices. I will present measurements of the electrical characteristics, the photovoltaic properties, and ultrafast spectroscopic studies of the carrier dynamics. Further, I will discuss atomically thin phototransistors, which show strong photoconductive gain. Finally, photocurrent generation studies in graphene and applications in optical communications will be presented. The focus of our work in this sub-field is on the 2D material integration into silicon chips for novel photonic integrated circuits. It is envisioned that the excellent material quality, combined with the advantages of 2D materials, such as flexibility, high mechanical stability and low costs of production, could lead to new electronic and optoelectronic technologies.

Spin-dependent electron scattering in 2D electron systems

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At the nanoscale electron scattering leads to well-known quantum effects such as quasiparticle interference and electron confinement. These were elegantly demonstrated with real-space visualization in the pioneering scanning tunnelling spectroscopy (STS) experiments using quantum resonators on metallic surfaces. Here, resonators of different geometry and chemical nature were artificially fabricated by moving atoms one by one [1], and later used as quantum laboratories for quantitative studies of scattering parameters [2,3], and for the exploration of more exotic phenomena such as the quantum mirage and invisibility [4,5].

Here I present STS studies that illustrate how the influence of exchange and spin-orbit coupling affects scattering of 2D electrons. In a first example I show how the Ni(111) exchange-split surface electrons undergo spin-dependent scattering at the interface with graphene, resulting in a total spin filtering effect [6]. The magnitude of the effect will depend on the atomic structure of graphene edges. The second example will focus on the electron confinement in 1D step resonators that are fabricated on Ag(111) and the $BiAg_2$ surface alloy, material with record-high Rashba-type spin-orbit interaction [7,8]. In the latter case, electrons are confined via a novel spin-flip mechanism originated by the spin-orbit locking, the strength of it being determined by the chemical composition of the steps. The two examples reveal fundamental phenomena that can be applied in future spintronics devices based on spinterfaces and spin-orbit textured materials.

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Simple Spintronics Devices Based on the Chiral Induced Spin Selectivity (CISS) Effect

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The high level of energy dissipation associated with the present semiconductor-based integrated-circuit technology limits the operating frequency of the devices. Therefore, there is interest in new concepts that may solve this problem. One such concept that attracts considerable attention nowadays combines spins with electronics (spintronics). In principle, the application of spintronics should result in reducing power consumption of electronic devices and efficiency should be closer to the thermodynamic limit. Two major issues complicate the use of spintronics; material problems and the inefficiency in producing spin-polarized current.

We present a new concept in which spin current is produced by using the spin selectivity in electron transport through chiral molecules, termed Chiral-Induced Spin Selectivity (CISS).[1,2] The CISS effect allows realization of simple local and power efficient spintronics devices. Studying the CISS effect, we found that chiral molecules, especially helical ones, can serve as very efficient spin filters at room temperature, with no need for a permanent magnetic layer. Recently, by utilizing this effect we demonstrated a simple magnetless optical and electrical magnetic memory[3,4] as well as local charge separation using a light induced configuration[5]. Moreover, we show that when chiral molecules are adsorbed on the surface of thin ferromagnetic film, they induce magnetization perpendicular to the surface, without the application of current or external magnetic field.[6]

The CISS-based spintronics technology has the potential to overcome the limitations of other magnetic-based memory technologies and to facilitate the fabrication of inexpensive, high-density memory and other spintronics elements.

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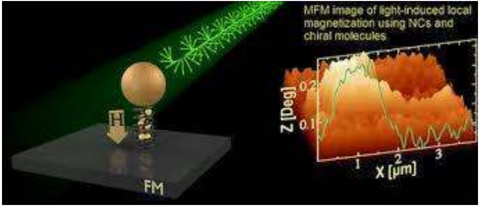
Figures



Determination of Structure of Nanoparticles by Small-Angle X-ray Scattering: Application to LDL Lipoproteins and to Refolding of SDS-Denatured Proteins

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Abstract: During the last two decades, there has been a tremendeous development of small-angle x-ray scattering (SAXS) instrumentation, at synchrotrons as well as at home sources. In particular the development of more powerful home sources and advanced optics means that even weakly scattering samples can be measured at home, and the commercialization of the instruments has led to a large increase in capacity, so that the use has become much more widespread. Simultaneous development of analysis and modelling methods means that more detailed structural information can be extraxted from the SAXS data. At Aarhus University we have in 2014 installed a SAXS instrument from Bruker AXS [1], which uses a powerful Ga metal jet X-ray source from Excillum, and which employs an optimized geometry with homebuilt scatterless slits [2]. In this contribution a recent application of this SAXS instrument for investigating the structure of low-density lipoprotein (LDL) particles [3] as a function of temperature will be presented. LDL is involved in atherosclerosis and the build-up of plaque inside the arteries, which is broadly involved in cardio-vascular deceases, the leading cause of death in the western hemisphere. In the work [3], a new model for determination of the structure of the LDL particles base on super ellipoids weas derived. The model allows fitting both size and shape, and also to determine the particular internal layering of the fats inside the LDL core. This gives in addition information on changes in the conformation of the protein component, which wraps the fatty core. The new approach allows a fast assessment of the structure which can be used routinely in research projects. This approach, now allows the monitoring of structural changes in the LDL upon different stresses from the environment, such as changes in temperature, oxidation, or external agents used or currently in development against atherosclerotic plaque build-up and which are targeting the LDL. In another project, protein-detergent interactions have been studied [4]. Globular proteins are usually unfolded and denatured by the anionic surfactant sodium dodecyl sulphate (SDS). This was also found for four investigated proteins, bovine serum albumin (BSA), α-lactalbumin, (αLA), lysozyme (LYZ), and β-lactoglobulin (βLG), which all form complexes, which are protein-decorated SDS micelles. Somewhat surprisingly, it was found that most of these proteins could be refolded by addition of the non-ionic surfactants (NIS), octaethylene glycol monododecyl ether (C12E8) and dodecyl maltoside (DDM). A relatively simple data analysis approach based on linear combination of SAXS data recorded for native protein, complexes, pure and mixed micelles, as well as mass conservation was employed. The addition of NIS to the protein-SDS samples resulted in extraction of the SDS from the protein-SDS complexes and refolding of βLG, BSA, and LYZ, while αLA changed to its NIS-bound state instead of the native state. It was conclude that NIS competes with globular proteins for association with SDS, making it possible to refold SDS-denatured proteins by adding sufficient amounts of NIS, unless the protein also has significant interactions with the NIS.

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Nano-Optomechanics with a levitated nanoparticle in vacuum

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Optomechanics holds great promises to push the limits of experimental physics, opening new opportunities in ultra-weak force sensing, thermodynamics and giving us further insight on the transition between the quantum and classical worlds. In this talk, we introduce the use of a levitated nanoparticle in vacuum as a nano-optomechanical system with unprecedented performances. We first describe its unique linear and nonlinear mechanical properties including its high sensing capability and bi-stable dynamics [1-3]. Subsequently, we present our efforts in cooling its motion towards mechanical ground state at room temperature. In particular, we report on an experiment that combines active parametric feedback cooling with passive resolved side band cooling in a macroscopic high finesse optical cavity [4,5]. Finally, we discuss how the concept of levitation optomechanics can be extended to optical nanocavity by exploiting their subwavelength mode confinement.

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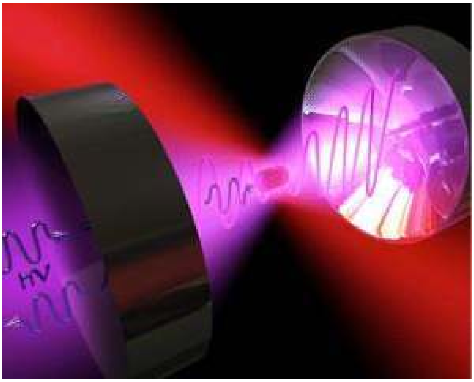

Figure1: Sketch of our experiment in which a levitated nanoparticle is cooled down by resolved side band cooling in a high finesse optical cavity.

Evaluation of the ecotoxicity and toxicity of graphene by a battery of multitrophic bioassays

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Currently, there are around nanomaterials a great interest due to their properties and the large number of applications they have. Nanomaterials are defined as naturals or manmade materials, which have at least one of their dimensions between 1 and 100 nm, while nanoparticles (NPs) include those with at least two dimensions between 1 and 100 nm. While research in nanotechnology and nanomaterials has come a long way, research on its effects on life and health has not yet reached the same level. In this context, the concept of nanotechnology is defined as the study of the adverse effects of nanoparticles on organisms, populations, communities and ecosystems. The urgency of these studies is driven by the rapid exploitation of known applications for nanotechnology for commercial and industrial entities. One of the most nanomaterials currently used are metal oxides.

The aim of this paper is to evaluate the ecotoxicity in one multilayer graphene in different environmental compartments and in human health, with the purpose of detecting at what levels, these particles can be harmful when they are released to the environment.

For these bioassay of acute toxicity, were performed in the organisms Daphnia magna, Selenastrum capricornutum, Vibrio fischeri and Eisenia fetida. Daphnia magna, a freshwater filter-feeding crustacean, is one of the most sensitive organisms used in ecotoxicity experiments. In addition to their sensitivity, their representation in the trophic level and its importance in the marine ecosystem are the reasons why this species is selected as indicator The trial follows the standard OECD 202 (OECD, 2004) Young daphnids, aged less than 24 hours at the start of the test, are exposed to the test substance at a range of concentrations for a period of 48 hours. Immobilisation is recorded at 24 hours and 48 hours and compared with control values. The evaluation of the acute toxicity in Eisenia fetida was performed following the instructions of the OECD 207 guide. Pseudokirchneriella subcapitata is a unicellular alga characteristic of lakes, rivers and freshwater ponds. To evaluate the toxicity of the materials in a kind of continental algae, was used the test Algaltoxkit FTM (MicroBioTests Inc., Gante, Bélgica). The test protocol provided by the manufacturer following the ISO 8692 standard and guide OECD 201. To evaluate the toxicity of the graphene in a detritivorous bacteria species was chosen Vibrio fischeri and was used the kit Toxi-Screening KitTM (MicroBioTests Inc., Gante, Bélgica). The test protocol provided by the manufacturer followed the ISO 11348-1 standard. Finally, a quantification of cellular and genetic damage was performed by a cell viability assay and the comet assay in epithelial cell line A459.

Figures

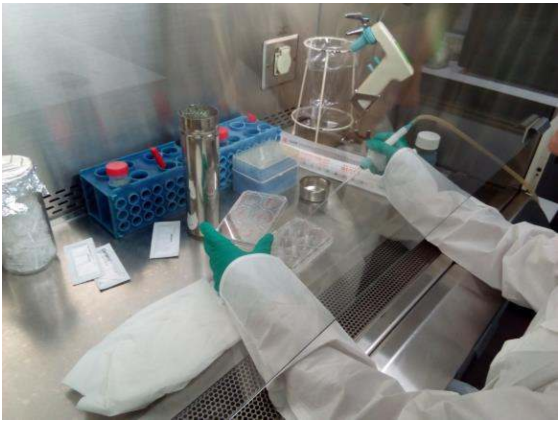

Figure 1: Cell Viability Assay

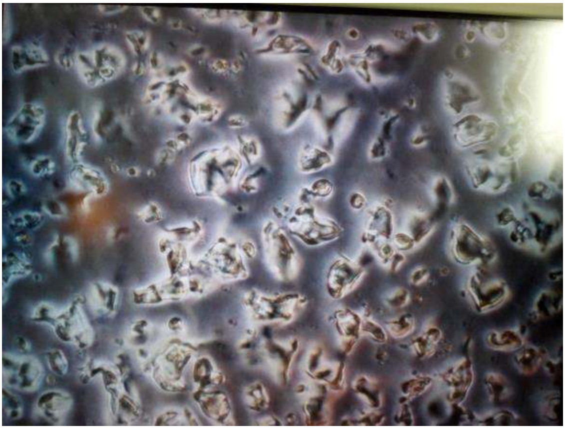

Figure 2: Cell Viability Assay

Fluorescent sensing probes based on GQDs immersed into Nanocellulose hydrogels

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Self-assembly of nanomaterials through reversible noncovalent forces is an excellent choice to fabricate responsive sensing probes. Attempts to incorporate fluorescent nanomaterials into gels were reported [1,2,3]. Our preliminary experience in the fabrication of gels has demonstrated that mixing an appropriate fluorescent system and a gelator [3,4] at the adequate proportions resulted in the formation of reversible transparent hydrogels; furthermore, the introduction of nanoparticles sometimes even accelerates the gel formation.

Herein, it is shown the simple preparation of fluorescent nanocellulose gels (Fig. 1) containing graphene quantum dots (GQDs) for sensing applications. This 3D network of nanodots assembled into nanofibers exhibits a significant enhancement of its photoluminescence properties as well as a strong sensing response towards several substances in comparison to those in solution.

The structural combination of fluorescent nanodots and nanocellulose hydrogels opens up new frontiers for nanomedicine inspired in biosensing, drug delivery and self-healing.

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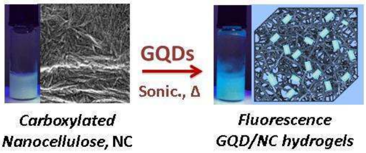

Figure 1: Fabrication of fluorescence hydrogels based on graphene quantum dots and nanocellulose.

(Intra)cellular therapies using magnetic and/or plasmonic nanoparticles : from thermal cancer treatments to tissue engineering and biotransformations.

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With the advent of nanotechnology in the field of medicine, new strategies have emerged to overcome some of the limitations of current cell therapies tools.

In cancer therapy, thermal treatments with magnetic or plasmonic nanoparticles provide noninvasive means of heating cells at therapeutic levels. While the ultimate target for nanoparticle-mediated thermal therapies is the cancer cell, heating performance was rarely evaluated intracellularly. In the attempt to bridge this gap, we provided thermal measurements mediated by magnetic [1] or plasmonic [2] nanoparticles inside cancer cells, in vitro or in vivo in the tumor environment. The ultimate goal of thermal cancer therapies is to improve the treatment efficacy and combat the tumour from within. We proposed combined nanotherapeutic concepts [3-5] based on magnetothermal, photothermal, and photodynamic therapies which led to complete cancer cell destruction in vitro and complete tumor ablation in vivo.

While magnetic nanoparticles are increasingly used as clinical agents for imaging and therapy, their use as a tool for tissue engineering opens up challenging perspectives that have rarely been explored. Our strategy has been to take advantage of magnetic nanoparticles internalization to create thick, organized, purely cellular 3D tissue structures [6,7], that can be stimulated on demand [8,9].

The use of nanoparticles for cancer cell therapies or tissue engineering raise more general issues of nanoparticles biosafety, once internalized in cells. Yet the nanoparticles long-term tissular fate is poorly documented. We have developed magneto-thermal techniques to follow the fate of magnetic and plasmonic nanoparticles and their assimilation within a living tissue [10,11].

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Figures

Figure 1: Magneto-photo-thermal approach in cancer therapy (left), magnetic tissue engineering (middle), and magnetic monitoring of tissular nanodegradation (right).

Oral contributions

Analysis of the robustness of Hierarchical hydrophilic and hydrophobic nanostructures

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From hydrophobicity to hydrophylicity different texture parameters have been analyzed on different polymer materials, like polycarbonate, cellulose acetate, COC, etc. The influence on the behavior of surface replicated features: pitch, diameter and height have been considered together with the different material properties, i.e. surface energy.

Changes in the hydrophobicity/ hydrophylicity behavior have been obtained by replication with adapted thermal nanolithography.

Robustness of the nanotextures has been analyzed for the different patterns as shown in the figures below.

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Figures

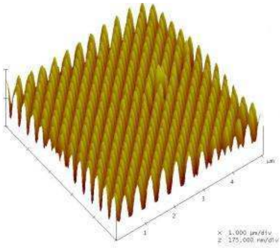

Figure 1: hydrophylicity texture replicated on CAB

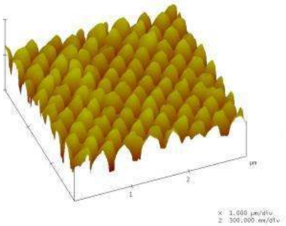

Figure 2: hydrophylicity texture replicated on CAB etched by NaOH

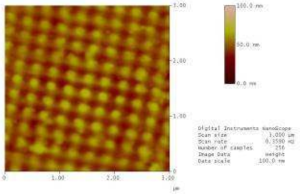

Figure 3: hydrophylicity texture replicated on CAB after soft mechanical stress

Metal Ferrite Nanoparticles and Toxicity to Normal and Cancerous Cell Lines

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Ferrite nanoparticles (NPs), with Copper and Cobalt, are important magnetic materials currently under research due to their applicability in nanomedicine. However, there is limited information concerning the interaction of such NPs with biological systems.

In several studies, we investigated the cellular response of both Copper and Cobalt ferrite NPs in human normal and cancer cell lines, such as breast cancer (MCF-7) and liver cells (HepG2). Cobalt ferrite NPs induced cell viability reduction and membrane damage, and degree of induction was dose- and time-dependent. They were also found to induce oxidative stress revealed by induction of ROS, depletion of glutathione and lower activity of superoxide dismutase enzyme. Overall, we observed that Cobalt ferrite NPs induced cytotoxicity and apoptosis in HepG2 cells through ROS via p53 pathway. Furthermore, biochemical studies showed that copper ferrite NPs induce cell viability reduction and membrane damage in MCF-7 cells and degree of induction was dose- and time-dependent. Also, Copper ferrite NP was found to induce oxidative stress in MCF-7 cells as indicated by reactive oxygen species (ROS) generation and glutathione depletion.

Further studies are underway to explore the toxicity mechanisms of metal ferrite NPs in different types of human cells. Our studies suggest that toxicity mechanisms of metal ferrite NPs should be further investigated in animal models.

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Figures

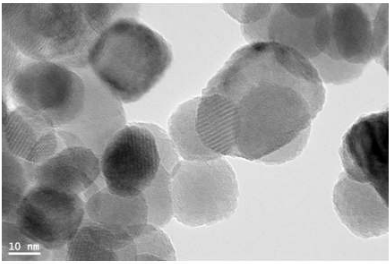

Figure 1: High resolution TEM image of copper ferrite NPs.

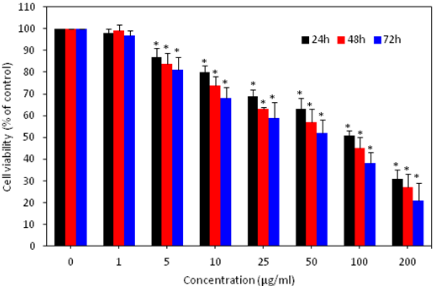

Figure 2: MTT assay of copper ferrite NP-induced cytotoxicity in MCF-7 cells at different dosages and exposure times. Data represented are mean±SD of three identical experiments made in three replicate. *Significant difference as compared to control ($p<0.05$).

Acoustic THz graphene plasmons revealed by photocurrent nanoscopy

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Abstract:
The interaction of terahertz (THz) radiation with graphene has a vast application potential in many technologies, including imaging, communications, sensing, or photo-detection, among others. Recently, it has been shown that the excitation of localized THz plasmons in graphene can strongly enhance light-matter interactions, opening the door to more efficient optoelectronic devices. Here, we will present on the first visualization of propagating graphene plasmons (GPs) at THz frequencies, which can also be controlled by metallic (split) gates. Intriguingly, due to the coupling of GPs with the metal gate underneath we observe a linearization of the plasmon dispersion (thus revealing acoustic plasmons), which comes along with an extreme confinement of the plasmon fields [1]. These extraordinary GPs properties are very promising for sensing and communication technologies. To map the THz GPs, we introduce nanoscale-resolved THz photocurrent nanoscopy as a novel tool for studying fundamental and applied aspects of local THz photocurrent generation with a resolution of 25 nm, nearly 4 orders of magnitude below the diffraction limit.

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Active Mid IR plasmonics using Giant Magneto Resistance

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Abstract

Plasmonics has proven as a powerful tool to improve the performance of mid-IR devices, resulting in plasmon assited quantum cascade lasers, plasmon enhanced light detection, plasmonic beam steering, plasmonic thermal emiters or plasmonic nanoantenas for vibrational spectroscopy. In this scenario, the possibility of modulating the emission, propagation and/or detection of mid-IR radiation constitutes a promising aspect to expand the limits of the currently used technologies. In this sense, fast and contactless actuation on plasmon resonances via the Magneto-Optical (MO) effect has been put forward by the inclusion of ferromagnetic components into noble metal layers and nanostructures, yet up to now restricted to the visible and near-infrared ranges.

Here we present our proposal and initial results on the magnetic field control of plasmon resonances in the mid IR region by the use of the Magneto-Refractive (MR) effect, i.e., a change in the optical properties of the system by magnetic field controlled electrical resistivity. For this we select a Giant Magneto Resistance model system (a Au/Permalloy multilayer), which exhibits changes in resisitivity of the order of 10% by the application of small (of the order of 20 Oe) magnetic fields. The experiments are carried out in a dedicated FTIR spectrometer with magnetic field capabilities.

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Figures

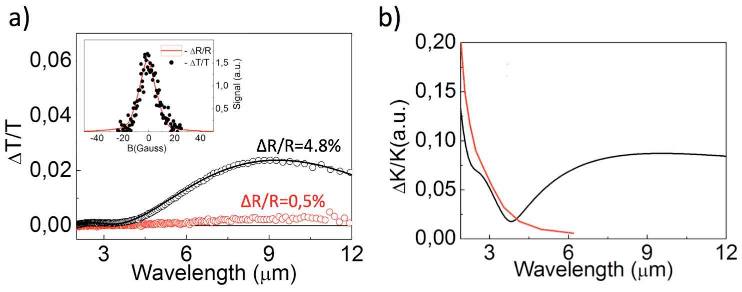

Figure 1: (a) Transmission spectra for two samples with different GMR values (4.8% and 0.5%). INSET: Magnetic field dependence of electrical resistance and integrated transmission in the mid IR region for the 4.8% GMR structure. (b) Calculated magnetic field modulation of propagating plasmons via MO effect (red) and MR effect (black). The modulation is similar for both MO and MR effects up to 3.5 μm, but it is much larger for the MR effect in the whole mid IR range.

Nanocomposites based on SBM triblock copolymer and Ag nanoparticles: morphological and dielectric analysis

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Nanocomposites based on polymeric matrix and inorganic nanoparticles present interesting properties, as the addition of inorganic functional nanoparticles endows the nanocomposite with specific advantageous optical, conductive, electric, or magnetic properties [1-3], for different potential applications such as photonic band gap materials, solar cells, sensors, and high-density magnetic storage devices [4, 5], among others. Among metallic nanoparticles, silver (Ag) ones are one of the promising candidates due to their unique optical, electrical and thermal properties and can be incorporated into products that range from photovoltaics to biological and chemical sensors. On the other hand, block copolymers are interesting platform to host those nanoparticles due to its ability to self-assembly into different nanostructures that can be used as templates.

In this work, thin film nanocomposites based on poly(styrene-*b*-butadiene-*b*-methyl methacrylate) (SBM) triblock copolymer and Ag nanoparticles have been prepared (from 0.5 wt% to 15 wt% nanoparticles), after modifying nanoparticles with dodecanothiol in order to improve their dispersion through the block copolymer. Good dispersion of nanoparticles has been obtained for all nanocomposites. Morphological characterization was carried out by atomic force microscopy (AFM), observing morphological changes promoted by nanoparticle addition (Figure 1). On the other hand, conductive properties of nanocomposites were analyzed by dielectric relaxation spectroscopy (DRS), concluding that all nanocomposites were below the percolation threshold.

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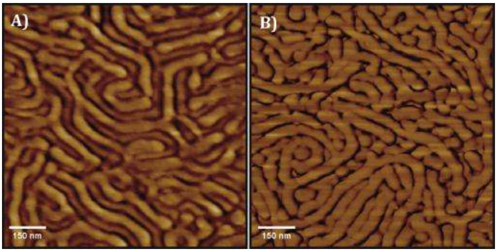

Figure 1: AFM phase images of thin films of (A) SBM and (B) nanocomposite with 5 wt% of Ag nanoparticles

Conductor films based on AgNWs spin-coated on glass substrates

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Silver nanowires offer the potential to make transparent coating with high electrical conductivity. In this study AgNWs formulations have been used in high volume spin deposition processes to create transparent conductor films with the following properties target:

Sheet resistance of 50Ω /sq and light transmission of >90%

The work has been focused on:

- Modify NWs concentration by diluting IPA-NWs dispersions, both in water and IPA
- Study the Ultrasounds effect in the NWs properties (electrical,optical…)
- Substrates treatment (wet and plasma etching) to improve the adhesion.
- Number of layers deposited on glass substrate

This study is financially supported by European Union´s Horizon 2020 (INSPIRED project).

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Figures

Ag/IPA:IPA	Layers	Substrate	Resistance	T%	Image
1:1	2	Soda Lime	50-70 Ω	74,72	
1:2	2	Soda Lime	66-70Ω	79,97	

Figure 1: Comparative values between two different AgNw disperssions.

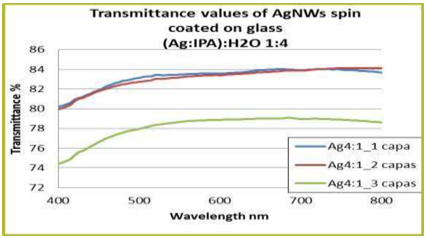

Figure 2: An example of transmission values of a concrete AgNw dispersion

New developments on Thermoelectric Materials: reducing scale and dimensionality

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Thermoelectric materials are able to convert a gradient of temperature in a diference of voltage, or vice versa. In order to improve the thermoelectric efficiency of these materials for actual applications, one of the most studied routes is the reduction in the dimensionality, via nanowire fabrication, for instance. This gives rise to a reduction of the thermal conductivity of the material due to the increase of phonon dispersion in the surface of the nanowires [1]. Another route to decrease the thermal conductivity would be the fabrication of interconnected three-dimensional structures, which could be seen as an intricate net of nanowires with many connection points, which increases the phonon dispersion and thus reduces the thermal conductivty.

We will review these kinds of structures along with the latest developments of template assisted electrochemical deposition of thermoelectric materials in three-dimensional templates. In this case, the reduction in thermal conductivity is due to the resulting interconnected three-dimensional structure that enhances the phonon scattering; compared with bulk, thin films or nanowires.

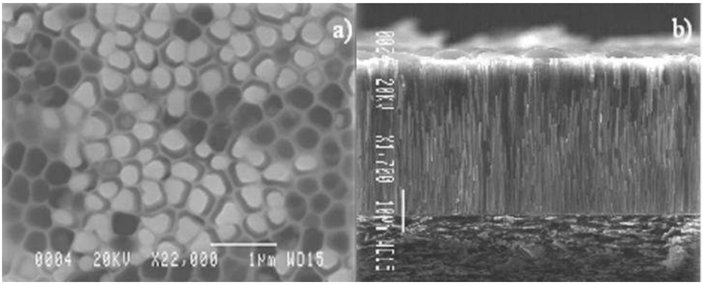

Fig1. SEM image of a) top view of an alumina matrix partially filled with Bi_2Te_3 nanowires (200 to 400 nm wire diameter) and b) cross section view of the same sample before polishing (taken from [2])

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Formation and characterization of perfluorocarbon nanocapsules as promising microbubble precursors for blood-brain barrier opening

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Microbubbles (MB) are used in the clinical field for a variety of applications such as ultrasound contrast agents, lithotripsy, etc. Recently it has been shown that MB can be used to open the blood-brain barrier (BBB) in a non-invasive, reversible and local manner when stimulated by focused ultrasound (FUS) [1, 2]. The preparation of suitable MB formulations is challenging, as they show short half-lifes and usually large and polydisperse particle sizes, which condition their biodistribution. In this context, nanocapsules containing a liquid perfluorocarbon which can phase shift to gas giving rise to expanded gas MB upon ultrasound stimulation are a promising approach [3].

The formation of polymeric perfluorocarbon nanocapsules prepared from nano-emulsion templates by the phase inversion composition method has been investigated in an aqueous solution / non-ionic surfactant / [polymer + non-fluorinated solvent + fluorinated solvent] system. It has been found that perfluorocarbon nano-emulsions can be formed at high oil-to-surfactant ratios and show sizes typically around 250 nm. Nanocapsules are obtained from the nano-emulsion templates by dialysis and show sizes below 150 nm. The presence of the highly volatile perfluorocarbon in the nano-emulsion template and further in the nanocapspules was confirmed by ^{19}F-NMR. The vaporization temperature of the perfluorocarbon once entrapped in the nanocapsules has been found to be higher (above 75ºC) than that of the no-encapsulated pure substance (around 58ºC). The as prepared perfluorocarbon nanocapsules show suitable features for their use as MB precursors.

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Multi-axial Evaporation trhough Nano-Hole Masks: a 3D-printer for the nanoscale

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Abstract

Nowadays we are witnessing breakthrough discoveries in science that improve our understanding of nature and put forward promising practical realizations. These discoveries very often benefit from nanofabrication techniques that allow obtaining sophisticated materials systems whose properties can be designed by structural and compositional control atdavid the nanoscale, making possible the exploration of novel physical phenomena unattainable up to day. Light-matter interaction is not an exception of this and, for example, magnetic field control and enhancement of this interaction have been demonstrated in nanosystems where building blocks with plasmonic and ferromagnetic properties coexist [1]. To give an example, by embedding a ferromagnetic nanodisk in a plasmonic ring and locating it below the hot spot of a plasmonic split ring, a three fold enhancement of the magnetooptical activity of the system can be achieved [2].

In this contribution we will show our developed strategy, based on the Hole Mask Colloidal Lithography technique[3] combined with multiaxial and multicomponent evaporation, to fabricate ensembles of 3D complex nanosystems over cm^2 areas. This has allowed us to obtain in the last years a diversity of magneto-plasmonic architectures with increasing degree of structural complexity and simultaneous in-plane (out-of plane) nanometer (subnanometer) control of the location and dimensions of the individual building blocks. This can be viewed as a nano-3D printer, with multiple cartridges corresponding to the different evaporation sources, the in-plane control being realized by the relative orientation of the hole mask template with respect to the evaporated material, and the out of plane control by the specific evaporation sequence. Examples will be shown on the fabrication of metal and metal-dielectric nanodisks, the corresponding morphologically complementary membranes, nanorods, nanorings and even more complex stacked ring-split / ring systems. They will also be illustrated with hints of their most relevant optical and magneto-plasmonic characteristics.

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Figures

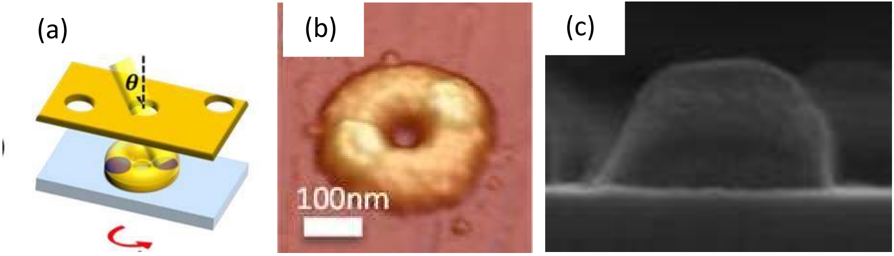

Figure 1: (a) Sketch of Au nanoring fabrication with Co inclusions (b) Corresponding AFM image in an intermediate fabrication step (H.Y.Feng, PhD Thesis) (c) SEM image of a metal/dielectric/metal magnetoplasmonic nanodisc.

Efficient Combination of Interference and Plasmon Resonance Raman Amplification by Optimized Heterostructures for Optical microscopy and Molecule Detection

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The detection, identification and quantification of different types of molecules and the optical imaging of, for example, cellular processes are important challenges. The enhancement provided by electric field amplification due to localized plasmons of metallic nanoparticles, called SERS (surface enhanced Raman scattering) is the most efficient process however, the design of amplification platforms for the detection and imaging of extremely diluted and/or complex materials still requires further research and development to get cheap, reliable, reproducible and stable over time systems that can be easily reused several times. Among the different mechanisms for Raman intensity amplification, the interference process has been scarcely investigated. Here we present how interference enhanced Raman scattering (IERS) in adequately designed heterostructures can provide amplification factors relevant both for detection and imaging. We report how interference enhancement substrates have to be designed to maximize their efficiency and how it is possible to combine SERS and IERS effects. The IERS platforms are demonstrated to improve significantly the quality of white light images of graphene and are foreseen to be adequate to reveal the morphology of ultrathin films and of biological material. We use a transfer matrix method to calculate the propagation of light through the heterostructure (reflecting layer/dielectric layer/graphene) [1] for a large set of materials in order to obtain the general trends of Raman interference process and to optimize the effect in view of its application. Graphene is used here as the ideal material to reveal the amplification power of the tested platform and as the appropriate substrate for the deposition of organic molecules. We have designed and fabricated optimized heterostructures for IERS which combined with nanostructured silver films demonstrate the combined IERS + SERS amplification.

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Hollow Gold Nanotubes with Controlled Length and Near-Infrared Absorption for Theranostic Applications

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Abstract

Important aspects in engineering gold nanoparticles for theranostic applications include the control of size, optical properties, cytotoxicity, biodistribution, and clearance. In this study, gold nanotubes with controlled length and tunable absorption in the near-infrared (NIR) region have been exploited for applications as photothermal conversion agents and in vivo photoacoustic imaging contrast agents. A length-controlled synthesis has been developed to fabricate gold nanotubes (NTs) with well-defined shape (i.e., inner void and open ends), high crystallinity, and tunable NIR surface plasmon resonance. A coating of poly(sodium 4-styrenesulfonate) (PSS) endows the nanotubes with colloidal stability and low cytotoxicity. The PSS-coated Au NTs have the following characteristics: i) cellular uptake by colorectal cancer cells and macrophage cells, ii) photothermal ablation of cancer cells using single wavelength pulse laser irradiation, iii) excellent in vivo photoacoustic signal generation capability and accumulation at the tumor site, iv) hepatobiliary clearance within 72 h postintravenous injection. These results demonstrate that these PSS-coated Au NTs have the ideal attributes to develop their potential as effective and safe in vivo imaging nanoprobes, photothermal conversion agents, and drug delivery vehicles. To the best of knowledge, this is the first in vitro and in vivo study of gold nanotubes.[1]

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Figures

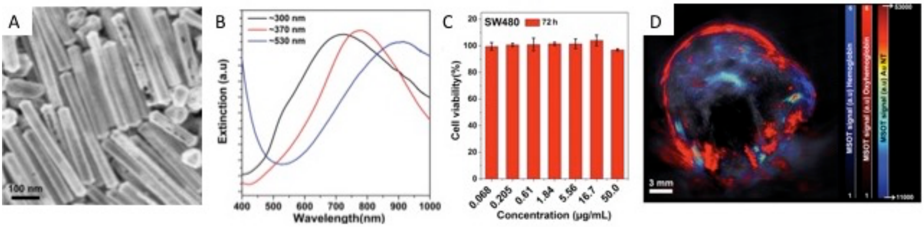

Figure 1: A. Hollow gold nanotubes of controlled length. B. NIR absorption, C) Cell viability assay and D) In-vivo imaging using Multispectral optical tomography.

The effect of PVP coatings on internalization and toxicological mechanisms of cerium oxide nanoparticles

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Abstract

Cerium oxide nanoparticles (CNPs, nanoceria) are increasingly used in industrial applications and may be released to the aquatic environment, where the exposure of aquatic organisms becomes likely. There are contradictory reports on whether nanoceria may act as an oxidant causing toxicity [1] or as an antioxidant being able to scavenge free radicals [2], given that the toxicological behaviour of these nanoparticles is still poorly understood. Moreover, little is known about the internalization process of CNPs in algae. There is evidence of CNP-internalization by *Chlamydomonas reinhardtii* (*C. reinhardtii*), but the internalization mechanism and route of uptake are still unknown [3]. In this study, we used an uncoated and different polyvinylpyrrolidone-coated CNPs (the purpose of the coating being to improve their stability, by inhibiting aggregation) with the aim of identifying their internalization and toxicological mechanisms. Monodispersed nanoparticles were synthesized and physicochemically characterized both in distilled water and the exposure media. Nanoparticles coated with PVP, irrespective of PVP molecular weight, provoked higher growth inhibition of *C. reinhardtii* than bare CNP. PVP-CNPs significantly increased ROS formation in exposed cells, indicating that oxidative stress might be an important toxicity mechanism. Interestingly, there was evidence of membrane integrity alterations which might facilitate further internalization of the nanoparticles. At present, the mechanisms of CNP-internalization are under thorough study.

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Understanding the Kinetics of Protein−Nanoparticle Corona Formation

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When a pristine nanoparticle (NP) encounters a biological fluid, biomolecules spontaneously form adsorption layers around the NP, called “protein corona”. The corona composition depends on the time-dependent environmental conditions and determines the NP’s fate within living organisms. Understanding how the corona evolves is fundamental in nanotoxicology as well as medical applications. However, the process of corona formation is challenging due to the large number of molecules involved and to the large span of relevant time scales ranging from 100 µs, hard to probe in experiments, to hours, out of reach of all-atoms simulations. Here we combine experiments, simulations, and theory to study (i) the corona kinetics (over 10−3−103 s) and (ii) its final composition for silica NPs in a model plasma made of three blood proteins (human serum albumin, transferrin, and fibrinogen). When computer simulations [1] are calibrated by experimental protein−NP binding affinities measured in single-protein solutions, the theoretical model correctly reproduces competitive protein replacement as proven by independent experiments. When we change the order of administration of the three proteins, we observe a memory effect in the final corona composition that we can explain within our model. Our combined experimental and computational approach is a step toward the development of systematic prediction and control of protein−NP corona composition based on a hierarchy of equilibrium protein binding constants [2].

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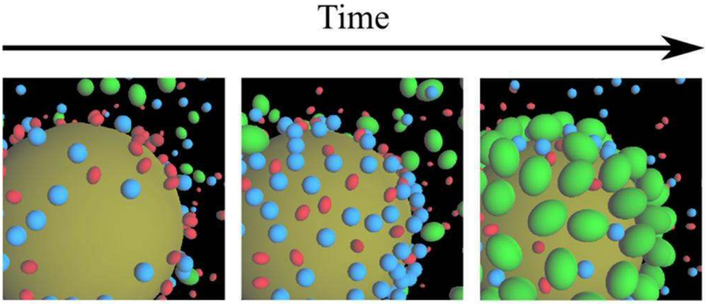
Figures



Kinetics of protein adsorption onto NPs.
Red: Albumin, blue: Transferrin, green: Fibrinogen.

Figure 1

An electronic beam splitter realized with crossed graphene nanoribbons

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Graphene nanoribbons (GNRs) are promising components in future nanoelectronics. We have explored a prototype 4-terminal semiconducting device formed by two crossed armchair GNRs (AGNRs) using state-of-the-art first-principles transport methods. 2 We analyze in detail the roles of intersection angle, stacking order, inter-GNR separation, and finite voltages on the transport characteristics. Interestingly, when the AGNRs intersect at $\theta = 60^{\circ}$, electrons injected from one terminal can be split into two outgoing waves with a tunable ratio around 50% and with almost negligible back-reflection. The splitted electron wave is found to propagate partly straight across the intersection region in one ribbon and partly in one direction of the other ribbon, i.e., in analogy of an optical beam splitter. Our simulations further identify realistic conditions for which this semiconducting device can act as a mechanically controllable electronic beam splitter with possible applications in carbon-based quantum electronic circuits and electron optics.

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Optical vortices in cilyndricaly symmetric all-dielectric optical scatterers

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The study of the optical response of high refractive index nano-particles has revealed that these resonant structures are capable of controlling different degrees of freedom of light fields with unprecedented versatility [1]. The ability of these particles to control the intensity, phase and polarization of light has unveiled a plethora of new physical effects. To mention a few, these particles have allowed controlling the directionality of optical antennas in an unprecedented manner [2], they have shown promise in enhancing chiro-optical spectroscopic techniques [3] and they have led to a generalized Brewster's condition to achieve full polarization of light [4].

In this letter, we unveil a new phenomenon that to the best of our knowledge was not reported up to date; the natural emergence of an optical vortex in the back scattering of cylindrically symmetric high index resonators when illuminated at their first Kerker condition of anomalous scattering. Firstly, based on singular optics arguments [5], we deduce the emergence of the vortex for a high index nano-particle Illuminated by circularly polarized light at the first Kerker condition. Secondly, using the recently developed helicity and angular momentum conservation framework [6], we prove that the modulus of the topological charge of the vortex has to be equal to 2. Lastly, we verify our predictions through analytic and numerical calculations.

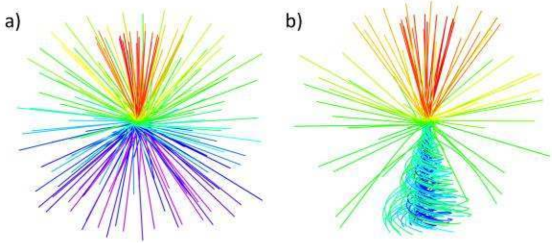

Figure 1: Poynting vector streamlines for the scattering of an all-dielectric scattererer illuminated by circularly polarized light when excited at; a) an arbitrary frequency, and b) at the first Kerker condition of anomalous scattering.

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Real-time Galectin Recognition by Dynamic SERS using Glycan-decorated Au Nanoparticles

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The monitoring of biomarkers, as indicators of physiological conditions, holds great promise as clinical diagnostics to facilitate successful treatment of diseases. [1] Most approaches in clinical diagnostics are accomplished using ELISA-based sandwich assays which are, however, time-consuming, tedious, and require experienced personnel. Efforts are still required at addressing these problems in the detection of biomarkers in real biological fluids. Surface-enhanced Raman scattering (SERS) is a promising surface-sensitive technology for assay readouts, [2] which offers simplified instrumentation, enhanced sensitivity and increased multiple analytical throughput.

Galectins are a family of galactoside-binding proteins that are found in multiple intracellular compartments and are secreted into the extracellular space. Altered expressions of galectins, usually increased, is commonly seen in pathological states, particularly inflammation, fibrosis, and regulation of various stages of cancers. [3] This research illustrates the use of SERS-active glycan decorated Au nanoparticles for the detection of galectins by surface enhanced Raman spectroscopy (SERS). The work presents an on/off SERS aggregation probe to investigate the multivalent carbohydrate-galectin interactions in real-time and in the use of SERS-active glyconanoparticles for the detection of galectins at nanomolar level in samples which mimic clinical biofluids. Additionally, the availability of portable Raman spectrometer testing these specific interactions is also demonstrated.

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Magneto-optical activity in high-index dielectric nanoantennas

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The control of light propagation in the visible and near-infrared domain using resonant systems such as optical nanoantennas has been a matter of intense research during the last decades. The possibility to create and manipulate nanostructured materials encouraged the exploration of new strategies to control the electromagnetic properties with an external agent. A possible approach is combining magnetic and plasmonic materials, where it is feasible to control the optical properties with magnetic fields in connection to the excitation of plasmon resonances [1].

These nanoantennas have been traditionally made of metallic entities, which have the important drawback of a sizeable absorption. In the case of magnetic resonances based on Babinet inverted magnetoplasmonic structures, it has already been demonstrated that the magneto-optical effect has the ability to manipulate magnetic dipole-like resonances [2].

In the last years, there has been a quest for the so-called magnetic resonances in the visible domain [3]. Linked to it, there has been an increasing interest in the use of high index dielectric nanospheres as optical antennas, in particular for their ability to sustain magnetic resonances and the absence of absorption [4-6]. In this work we introduce the magneto-optical effect in the context of those high index dielectric nanospheres, i.e. a silicon nanosphere with a non-negligible of diagonal element in the dielectric tensor. We will show how the magneto-optical effect is controlled by the internal resonances of the nanosphere, and that the magnetic resonances dominate the spectral dependence of the magneto-optical response, having the electric dipolar resonance a very weak effect. We will establish a clear correlation of the spectral magneto-optical response with the spatial field profile at the interior of the nanosphere that is, in turn, linked to each type of resonance [7].

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Probing low-energy hyperbolic polaritons in van der Waals crystals with an electron microscope

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Van der Waals materials (vdW) are a wide class of 2D systems in which individual atomic layers are only weakly bound by van der Waals interaction [1]. Much of the vdW materials functionality results from the large anisotropy in the bonding strength of atoms in the direction parallel to atomic layers and across them, and is often intimately connected with the corresponding phonons. The investigation of phononic excitation in vdW materials thus requires low mid-IR energies with nanoscale spatial resolution. Electron energy loss spectroscopy performed in scanning transmission electron microscopy (STEM-EELS) is a versatile technique capable of performing spectroscopy at the nanoscale [2]. However, conventional STEM-EELS has limited capabilities for mid-IR spectroscopy primarily due to poor monochromaticity of the primary electron beam and limited resolution of the detection system, which mask low energy excitations below 200 meV with the zero loss peak (ZLP) originating from the elastic electron scattering.

Here, we reduced the ZLP width of a conventional STEM-EELS system down to 50 meV which allowed us to probe low-energy phononic excitations (down to 100 meV) in vdW materials. Particularly, we performed a nanoscale mapping of electron energy loss (EEL) in hBN flakes, a representative vdW material. Surprisingly, we observe a variation in EEL peak position as a function of flake thickness and the edge prximity, which can not be explained by the bulk phonon excitations. Instead, our developed theory reveiles that the energy loss is dominated by the excitation of phonon polaritons, which exhibit a hyperbolic dispersion [3] owing to the layered crystal structure of hBN. The propagating nature of these hyperbolic polaritons explains the observed phenomena and suggests that STEM-EELS is highly suitable for the investigation of optical/polaritonic properties of vdW materials, with our work laying the foundation for such investigations. With ongoing developments in the monochromator and electron gun designs, we expect further improvement of STEM-EELS spectral resolution and the applicable energy ranges in near future, allowing for correlative studies of polaritons and structural properties in vdW materials.

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Figures

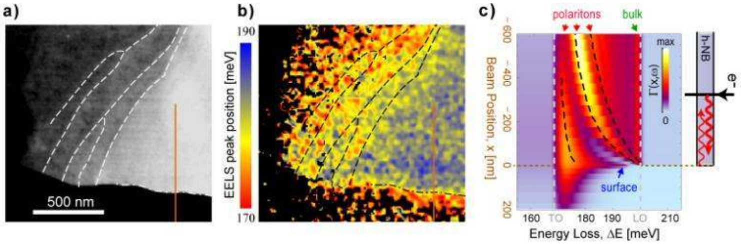

Figure 1: (a) HAADF image of hBN flake. (b) EELS peak position map. (c) Calculated EELS probability profile (along the brown line in panels a and b) reveiling the dominant role of hyperbolic polaritons.

Macroscale Construction of Plasmonic 3D Supercrystals *via* Templated Assembly of Monodisperse Gold Nanospheres

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Ordered arrangements of plasmonic nanoparticles are crucial for a plethora of intriguing technologies such as optical metamaterials, subwavelength light management, or ultrasensitive molecular detection.[1,2] For three-dimensional assemblies, the most common building blocks are gold nanospheres, which can form supercrystals with face-centered cubic (fcc) or hexagonal close-packed (hcp) lattices in dense packing. Hereby, despite much progress in the assembly of small mesostructures, preserving ordered packing in large supercrystals remains a major challenge demanding both exceptionally regular particles as well as reliable assembly techniques.[3,4]

In this contribution, we present solutions for these two important aspects. First, a facile protocol is introduced yielding gold nanoparticles that are not only monodisperse in size but also remarkably spherical and rounded: hereby, growing the particles quickly to the desired size and removing surface roughness subsequently by an efficient etching procedure enabled the synthesis of large quantities of well-defined nanospheres with diameters up to 110 nm. Second, we discuss the arrangement of nanospheres into pyramid-shaped supercrystals by template-assisted self-assembly: after PEGylation and partial removal of the stabilizing surfactant these gold nanospheres could be utilized to build arrays of separated pyramids by simple drying of highly concentrated dispersions between a topographically structured, hydrophobic stamp and a flat hydrophilic target substrate. Thereby, uniform pyramid assemblies were obtained over mm^2 areas. Investigation by high magnification SEM and focused ion beam cutting through individual square base pyramids showed that the nanospheres assembled into an fcc lattice forming high-quality, micron-sized supercrystals.

Our results represent a facile pathway enabling the large-scale assembly of highly organized plasmonic supercrystals, which is of special importance for functional materials with applications, for instance, in light harvesting and sensing.

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In Situ Determination of Colloidal Gold Concentrations with UV–Vis Spectroscopy: Limitations and Perspectives

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The Au(0) concentration in a gold nanoparticle (GNP) solution represents an important information. However, its exact determination often remains a major issue but is crucial for biological applications and their related toxicological discussions. Moreover, for investigations of GNP formation mechanisms, various GNP surface modifications and particle assembling procedures, accurate Au(0) concentration values are required.

In this work the UV–vis absorbance of colloidal gold nanoparticles at 400 nm is studied and validated as a method to determine Au(0) concentrations in GNP solutions. The method is shown to be valid with restrictions depending on the investigated system. The uncertainty of the determined Au(0) concentration can be up to 30%. This deviation is the result of the combined influence of parameters such as particle size, surface modification, or oxidation state. However, quantifying the influence of these parameters enables a much more precise Au(0) determination for specific systems. As an example, the reduction process of the well-known Turkevich method (citrate reduction) was monitored and the Au(0) concentration was determined with a deviation of less than 5%. Hence, a simple, fast, and cheap in situ method for Au(0) determination in GNP solutions is demonstrated that has in the presence of other gold species such as Au(III) an unprecedented accuracy.

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Figures

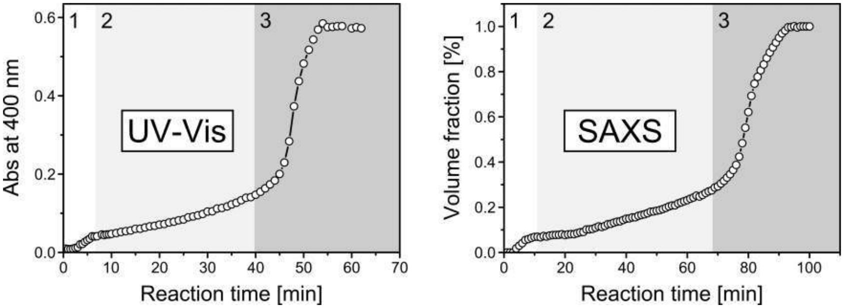

Figure 1: Left: Time-resolved UV−vis measurements of the absorbance at 400 nm for a GNP synthesis using citrate reduction. Right: The results are compared to the volume fraction derived from SAXS measurements.

Tunable Nanoparticle and Cell Assembly Using Combined Self-Powered Microfluidics and Microcontact Printing

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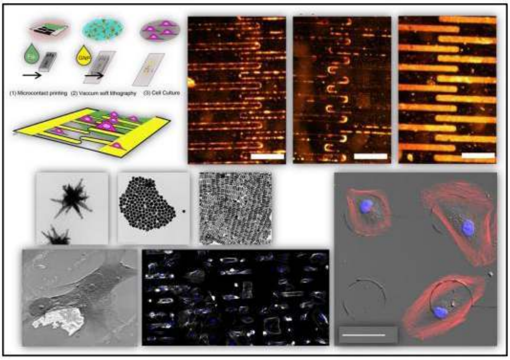
The incorporation of nanomaterials in biomedical devices is becoming increasing common in regenetative medicine, *in vivo* based scaffolds and for the production of organ-on-a-chip type devices. In this context, we designed a device in which we have nano-scale control over the location of inorganic nanoparticles (NP) and proteins on a substrate.

We used a combination of “degas-driven flow” and a microfluidic device to initiate the controlled deposition of different shaped and sized gold NPs on a substrate. This vacuum-soft lithography could be used to produce different NP organisations including nanowires, NP layers, and 3D supercrystals. The morphologies were dictated not only by the mould (a PDMS template) but also by the surface chemistry of the NPs. We combined this technique with microprinting for deposition of biomolecules on, or around, the nanostructures. The approach, named “Printing and Vacuum (PnV) lithography”, allowed a wide choice of type and distribution of NPs and biomolecules.

We used these substrates to show control over the deposition and growth of various human cells, including healthy endothelial and cancerous cells, reacting to both NP supercrystal morphology and biomolecule deposition. Such substrates were non-toxic and cells remained viable over days. Various methods could be used to “view” the proceses occurring from the initial NP deposition on the substrate (darkfield microscopy) to cell interactions with underlying biomolecules (surface enhanced Raman spectroscopy), and individual cell:NP connections (SEM). We obtained preliminary results in the use of plasmonic gold NPs to induce local heating and manipulation of cell adhesion.

In conclusion, we present a noval multicomponant patterning technique which can act as a biocompatible substrate for controlled cell morphology and function.



Clay-Metal Hybrid Nanoparticles towards Plasmonic Materials

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Clay minerals are abundant natural materials arising in the presence of water, which are ubiquitous on earth and even on other planets such as Mars. In addition to their abundance and low cost, properties of clays such as high surface area, good ion-exchange capacity, and recyclability have led to their widespread use in industrial processes. The interlamellar space between layered silicate clays can also be used to host a variety of different organic and inorganic guest molecules or particles, which has been shown to be a promising strategy for the loading of drug and dye molecules. Following this line of interest, a method for the seedless synthesis of gold nanoparticles on the synthetic layered silicate clay Laponite was developed. This facile approach can be used to make metal-silicate nanoparticles with a variety of morphologies, with potential applications in plasmonic sensing, catalysis, and novel composite materials.
ONE page abstract format: including figures and references.

References

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Figures

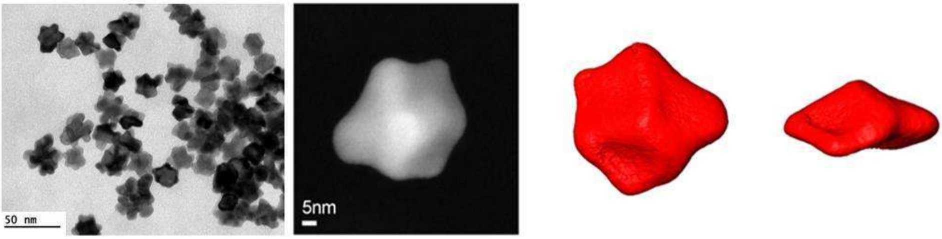

Figure 1: TEM images and 3-d reconstructions of laponite-gold nanoparticles

Understanding the Surface of CdSe Semiconductor Nanocrystals with Computational Chemistry

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Colloidal semiconductor nanocrystals (NCs) are characterized by a large surface-to-volume ratio that renders them extremely sensible to processes occurring on the surface.[1] The capping ligands, used to stabilize the nanocrystal in an organic solvent, play an important role in influencing the structure and the optoelectronic properties of these materials.

Despite major progresses to characterize the chemical reactions occurring on the surface of CdSe NCs, there are still several key questions to be answered on the nature of the NC-ligand interactions and how trap states, which are deleterious for charge transport, are formed on the surface.[2]

A leap forward in solving the above issues is to analyze the surface using theoretical simulations. Based on a combination of Density Functional Theory and Molecular Dynamics simulations, we present the first multiscale modeling of real sized CdSe QDs (about 4.0 nm) capped with oleate ligands and immersed in an organic solvent like dichloromethane with a simulation box containing 25000 atoms.[3] Molecular dynamics simulations, carried out up to the microsecond timescale, provide crucial insights on the surface dynamics, and the role of the ligands on the structural optoelectronic properties of these materials.

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Figures

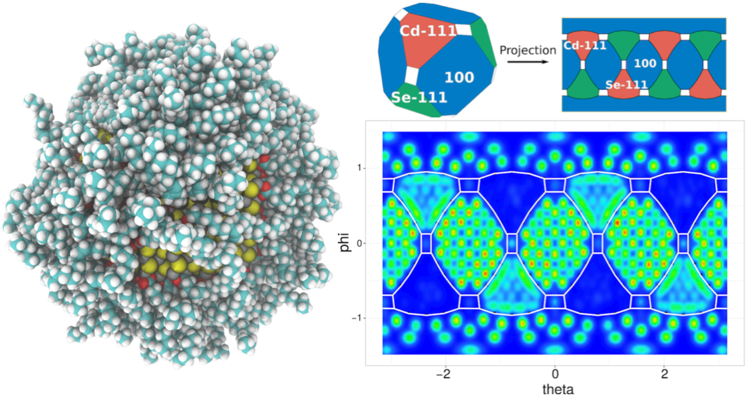

Figure 1: (left) Modelled CdSe NC; (right) Ligand distribution on the NC surface projected on a 2D plane.

Investigating Cell-Substrate and Cell–Cell Interactions by Means of Single-Cell-Probe Force Spectroscopy

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Cell adhesion forces are typically a mixture of specific and nonspecific cell-substrate and cell–cell interactions. In order to resolve these phenomena, Atomic Force Microscopy appears as a powerful device which can measure cell parameters by means of manipulation of single cells. This method, commonly known as cell-probe force spectroscopy, allows us to control the force applied, the area of interest, the approach/retracting speed, the force rate, and the time of interaction. Here, we developed a novel approach for in situ cantilever cell capturing and measurement of specific cell interactions. In particular, we present a new setup consisting of two different half-surfaces coated either with recrystallized SbpA bacterial cell surface layer proteins (S-layers) or integrin binding Fibronectin, on which MCF-7 breast cancer cells are incubated. The presence of a clear physical boundary between both surfaces benefits for a quick detection of the region under analysis. Thus, quantitative results about SbpA-cell and Fibronectin-cell adhesion forces as a function of the contact time are described. Additionally, the importance of the cell spreading in cell–cell interactions has been studied for surfaces coated with two different Fibronectin concentrations: 20 µg/mL (FN20) and 100 µg/mL (FN100), which impact the number of substrate receptors.

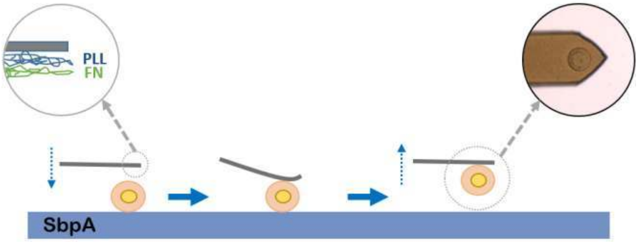

Figure 1: Schematic cell capturing process: the chemically modified flat cantilever is placed in contact with an individual MCF7 cell which stands on top of the SbpA-coated substrate.

PLAMONIC NANOPARTICLES IN ORGANIC SUSPENSIONS: PHASE TRANSFER AND APPLICATIONS

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Plasmonic nanoparticles are key building blocks with unique features that allow exploitation of light-matter interactions across different fields.[1,2] Since the optical properties of plasmonic nanomaterials are directly related to their morphology, much effort has been devoted to develop synthetic routes toward the preparation of these materials. Although the preparation of anisotropic nanoparticles with accurate size and shape control is mainly carried out in water, stable nanoparticles in organic solvents are required for several applications. In this context, we present a general route for the phase transfer of plasmonic nanoparticles of different shapes and sizes.[3] The obtained stable organic dispersion can be then used for different applications: Taking advantage of the excellent spreading of such organic dispersions on water, self-assembly of nanoparticles was achieved at the air/liquid interface, leading to extended nanoparticle arrays that could be in turn transferred onto solid substrates to obtain homogeneous plasmonic substrates.

Additionally, the obtained hydrophobic nanoparticles could be further coated with an amphiphilic polymer, which provides the advantage to disperse nanoparticles in biological media with high physiological stability and biocompatibility.[4] Furthermore, using hydrophobic Raman reporter molecules to transfer the particles, that concomitantly act as capping agents, efficient SERS-encoded nanoparticles for multiplexed cell discrimination can be obtained. These tags were used to distinguish five different types of breast cancer cells by imaging of a quintuple cell co-culture.[5]

Plasmonic nanoparticles suspended in organic media can also be included into bicompartmental polymeric particles produced by electrohydrodynamic co-jetting technique.[6] These biodegradable particles can be used for controlled drug delivery or cell and/or scaffold labelling in long term experiments.

We have demonstrated that this general method to obtain plasmonic nanoparticles in organic suspensions offers new opportunities for future applications.

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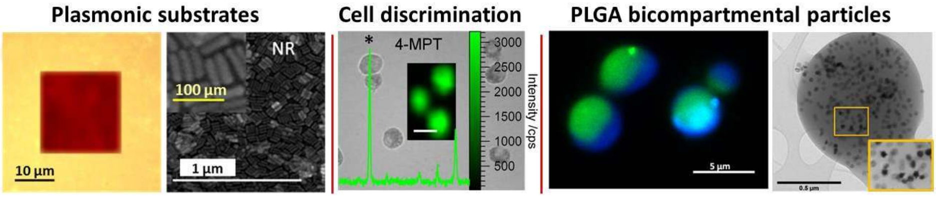

Figure 1: Applications of plasmonic nanoparticles in organic suspensions

Cell-Detachment from Plamonically Active Polyethylene Terephthalate (PET) Subtrates by Application of Near-Infrared Light

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Cell culture is a multibillion dollar industry with applications in a wide range of fields. Currently there is a need for cheap, efficient and non-damaging methods to detach cells from cell culture substrates. Plasmonically active gold surfaces are particularly useful in this regard as they can be utilized to efficiently induce cell detachment via the application of near-infrared light.[1] In this work, PET substrates have been rendered plamonically active with the aim of fabricating cell culture device. Arrays of gold nanoseeds have been formed using block co-polymer micelle nanolithography and from these, anisotropic gold nanostructures have been grown via the reduction of gold chloride in solution. The resulting substrates show broad plasmon bands in NIR region of light as evidenced by UV spectroscopy. HeLa cells have been successfully grown on these substrates and detached under the application of 980 nm light. Once the conditions for the efficient detachment of a wide variety of cells has been determined it is planned that this process will be scaled-up to allow existing cell culture devices, such as T-flasks and roller bottles, to be rendered plamonically active for facile cell harvesting post cell-culture. Furthermore, additional methods to fabricate plasmonics surfaces using alternative cell culture substrates will be explored.

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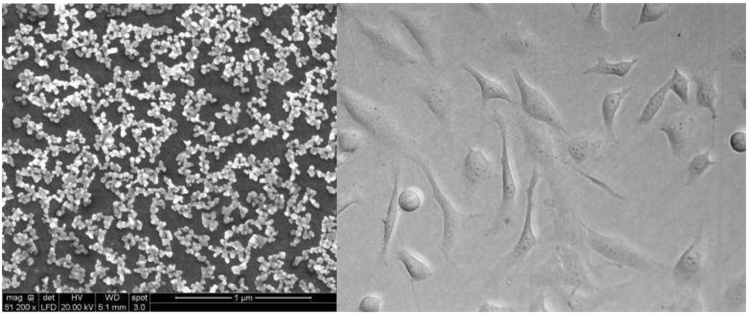

Figure 1: SEM image of anisotropic gold nanostructures grown on PET (left). Optical microscopy image of HeLa cells grown on plasmonically active PET substrates (right).

Scanning Microwave Microscopy for Complex Material Characterization

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Scanning Microwave Microscopy (SMM) is a recent development as a nanoscale imaging technique that combines the lateral resolution of Atomic Force Microscopy (AFM) with the high measurement precision of microwave analysis at GHz frequencies. It consists of an AFM interfaced with a Vector Network Analyzer (VNA) with operating frequencies ranging from 1 to 20 GHz.

SMM allows measuring complex materials properties for nano-electronics, materials science - photovoltaics and semiconductors - and life science applications.

Here we present the basic working principles of SMM and its advanced applications. In particular, the capabilities of the SMM include: calibrated capacitance and resistance measurements with a noise level of 1 aF [1]; a 2D mapping workflow to acquire roughly 20.000 C-V curves during one image [3]; calibrated complex impedance imaging of semiconductor [2], dielectric [6, 7], and biological [9, 10] samples; point wise C-V (capacitance-voltage) spectroscopy curves allowing for oxide quality characterization, interface traps, and memory effects of novel materials.

Due to the fact that microwaves can travel and penetrate into materials, SMM has been used already for 3D tomography applications of semiconductor structures [7, 8], examples include charge redistribution monitoring or composite material quality control measurements. A new way is paved to non-destructive sub-surface imaging in material science (see figure 1).

Recently, calibrated complex impedance images of cells and bacteria have been obtained with the SMM [9, 10], proving that this method also works in liquid environments like buffer solutions.

Experimental investigations are complemented by finite element radio-frequency modelling using the 3D architecture of the probe and the sample, done with the Keysight software EMPro [4, 5].

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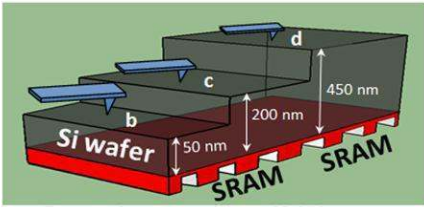

Figure 1: Sub-surface imaging of an SRAM (static random access memory) device, imaged with AFM on the backside of the p- and n-dopant lines of the SRAM structure. Microwaves originating from the scanning AFM tip in SMM mode easily permeate the oxide layers and thereby allow us to quantitatively determine dopant levels underneath the surface.

Efficient G_0W_0 using localized basis sets: a benchmark for molecules

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Electronic structure calculations within Hedin's *GW* approximation are becoming increasingly accessible to the community. In particular, as it has been shown earlier and we confirm by calculations using our **MBPT_LCAO** package [1], the computational cost of the so-called G_0W_0 can be made comparable to the cost of a regular Hartree-Fock calculation. In this work, we study the performance of our new G_0W_0 implementation (based on a contour deformation technique) to reproduce the ionization potentials of all 117 closed-shell molecules belonging to the G2/97 test set (see figure below), using a pseudo-potential starting point provided by the popular density-functional package **SIESTA** [2]. Moreover, the ionization potentials and electron affinities of a set of 24 acceptor molecules [3] are compared to experiment and to reference all-electron calculations.

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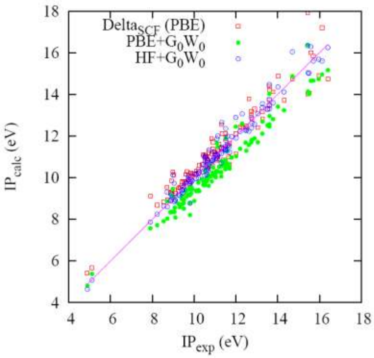

Figure 1: Ionization potentials of G2/97 test set computed with Delta SCF, and PBE+G_0W_0, and HF+ G_0W_0. HF+ G_0W_0 shows a least deviation from experimental data.

Physics of turbomolecular pumps and demonstration of conductance influence in HV

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The turbomolecular pump, a further development of the early molecular drag pump first introduced by Wolfgang Gaede in 1913 [1], is a high-vacuum (HV) pump which is used both for attaining very low ultimate pressures down to 10^{-10} mbar and for handling of high process gas flows up to inlet pressures of 10^{-2} mbar. The rich variety of high-vacuum applications requires a rich variety of high-vacuum pump designs. In particular, high-vacuum pumps have to handle gases with significantly different thermodynamic properties, they have to perform in the wide pressure regime mentioned above, and they have to perform at tremendously different gas throughputs. Before the development of a turbomolecular pump starts it is imperative to decide whether the pump design should be optimized for high compression ratios or for high pumping speeds.

First and foremost, the requirements with regard to ultimate total pressure (= compression ratios) and gas type-specific pumping speeds at certain inlet pressures determine the design of the inlet flange and hence, the dimensions of the pump, the design of the rotor and electric motor as well as the choice of the bearing concept.

Nowadays, there are two designs of turbomolecular pumps which are of commercial interest:

- The “classic turbomolecular pump”first described by Willi Becker in 1958 [2].
- The “compound turbomolecular pump” developed and optimized in the 1980s.

Both designs will be shortly presented highlighting the specific advantages and disadvantages.

Besides the performance of the turbopump itself there are several factors which influence the final performance of the vacuum system. Basic rules to obtain low pressures and fast pump down will be presented briefly. Those rules cover a suitable chamber design with minimized surface area, selection of appropriate materials as well suitable pre-treatment of materials and surfaces for HV conditions.

All fixtures between intake of pump system and chamber will lead to a reduction of pumping speed. This effect is described with the conductance C. The conductance is pressure dependant and has a strong influence in HV and UHV conditions. The conductance also depends on the geometry of the fixtures. Some basic guidelines to avoid conductance losses will be presented.

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Figures

Figure 1: On the left: Classic turbomolecular pump; on the right: compound turbomolecular pump fitted with three Holweck stages in series

Optical cell imaging with plasmonic nanomaterials

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The vibrational fingerprint of a molecule not only reflects its geometrical structure (configuration/conformation) but also reveals intermolecular or molecule-surface interactions and orientations. In this context, surface-enhanced Raman scattering (SERS) becomes a very popular tool in optical analytics due to broad application combined with ultra-sensitive detection potential down to single-molecule limit [1]. Imaging of cells by means of SERS-labeled nanoparticles as tags is an efficient strategy when direct detection is under the threshold, e.g., due to the low Raman cross section of many biomolecules. The properly tailored nanotag can offer multitasking or multiplexing capability including interrogation of processes as cell/nanoparticle tracking, drug delivery, nanoparticle fate etc.

In this work, we present a few examples of *in vitro*-SERS imaging for several cell types using different nanoparticle designs. We used (i) highly stable, encoded gold nanostars (AuNS) for cell type assignment at long-time scales to study evolution and stability of co-culture samples [2], (ii) AuNS-polystyrene (PS) bead assemblies with multimodal imaging potential via correlated fluorescence-dark-field-SERS spectroscopy[3] and (iii) double-encoded Janus particles as model for color-sensitive single component or duplexed detection of [4].

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Figure

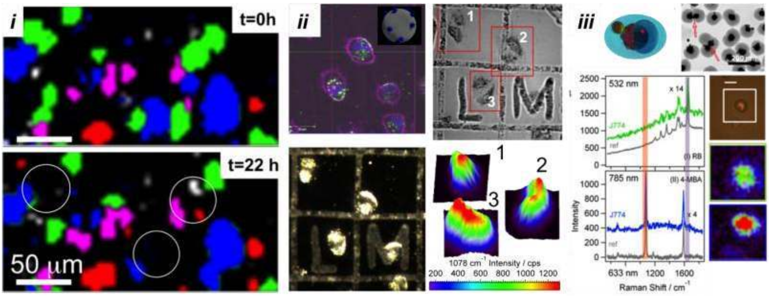

Figure 1: *i)* Evolution of a quintuple breast cancer cell culture with differently encoded AuNS, *ii)* correlated fluorescence-dark-field-SERS imaging of A549 with 4-mercaptobenzoic acid (4-MBA) labeled AuNS-PS beads and *iii)* color-sensitive detection of rhodamin B or 4-MBA in J744 with Janus particles.

Nanostructured Bioactive Polymeric Layers for Trapping DNA and Proteins

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The present study strongly relates to ongoing research on the development of cationic (anionic) polymers which are of great interest due to their enormous potential for biomedical applications, especially as non-viral vectors for gene therapy, antimicrobial agents and active components in DNA (protein) sensing devices [1]. We demonstrated that a functional group approach can be successfully realized in a free-radical copolymerization process to prepare cationic copolymers with a desired composition of bioactive functional groups, which can be activated in water thus, providing electrostatic interactions between a polycation(anion) and DNA (protein) [2, 3].We developed a protocol of the film casting, which permits to reproducibly prepare bioactive films with regular cavity-like nanostructured surfaces. The proof-of-concept experiments demonstrated the capabilities of these nanovcavities to trap single DNA (protein) molecules (Fig. 1 and 2).

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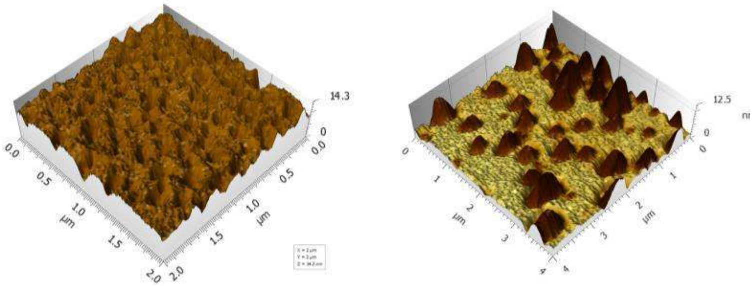

Figure 1: 3D rendered images of the topography information and bimodal colors of cavity-like nanostructured surfaces: left, as prepared cavities and right, cavities fitted with mioglobine. Roughness is topography while the colors is the surpimpossed image of Bimodal phase

The SIESTA Code: Basis Set Construction Strategy. Comparing Solid State DFT Codes

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Abstract

SIESTA is both a method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.[1] In the SIESTA code, finite-support atomic orbitals are used as basis set.[2] In this work we have designed a basis set construction strategy to generate efficient basis set. The optimization target has been the minimization of the average energy of a set of Ndi symmetric dimers at different bond distances (di).

The reproducibility of results is one of the underlying principles of science. In spite of the absence of one absolute reference code, the reproducibility of DFT results can be established by a broad and comprehensive test for precision; Δ-DFT test. [3] As a second stage of this project, the original Δ-DFT protocol will be applied to the SIESTA method firstly to test the quality of the newly generated basis, and secondly to demonstrate SIESTA competitiveness against other codes. Applying the Δ-DFT test, the precision is assessed by means of a pairwise comparison of a wide range of codes and methods respect to their predictions of the equations of state of the elemental crystals. This test has already been performed for more than ten atomic-scale simulation codes with characteristics similar to SIESTA code (WIEN2k, GPAW, VASP, ABINIT, etc.).

After the Δ-DFT test is successfully completed, the basis set database generated in this project will be incorporated into the software SIESTA PRO. SIESTA PRO, computer program currently developed by SIMUNE (www.simune.eu), has the aim to automatize and increase the efficiency of the use of the SIESTA code.

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Poly(methacrylic acid)-based single-chain polymer nanoparticles for targeting and imaging pancreatic tumors *in vivo*

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Cancer accounted for 8.2 million deaths worldwide in 2012 and, for some types of cancer, e.g. pancreatic adenocarcinoma incidence equals mortality [1]. The development of tools for the early diagnosis of pancreatic adenocarcinoma is an urgent need in order to increase treatment success rate and reduce patient mortality.

Here, we present a modular nanosystem platform integrating soft nanoparticles with a targeting peptide and an active imaging agent for diagnostics. Biocompatible single-chain polymer nanoparticles (SCPNs) based on poly(methacrylic acid) were prepared and functionalized with the somatostatin analogue PTR86 as the targeting moiety (Figure 1), since somatostatin receptors are overexpressed in pancreatic cancer.

The gamma emitter ^{67}Ga was incorporated by chelation and allowed *in vivo* investigation of the pharmacokinetic properties of the nanoparticles using single photon emission computerized tomography (SPECT). The resulting engineered nanosystem was tested in a xenograph mouse model of human pancreatic adenocarcinoma. Imaging studies demonstrated that accumulation of targeted SCPNs in the tumor is higher than that observed for non-targeted nanoparticles due to the improved retention of the nanocarrier in this tissue [2].

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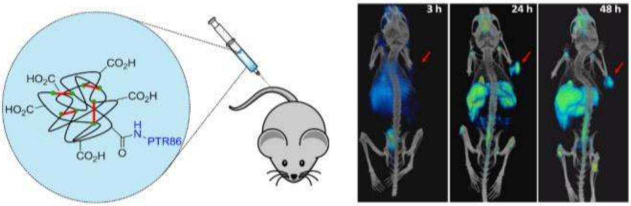

Figure 1: Water dispersible, radiolabeled and targeted single-chain poly(methacrylic acid) (PMAAc) nanoparticles were injected into mice bearing subcutaneous human pancreatic ductal adenocarcinoma. Imaging studies were performed *in vivo* by SPECT at different times.

Overcoming autofluorescence: long luminescence lifetime nanoparticles for time-gated bioimaging

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The applicability of fluorescence for in vivo imaging is often hampered by the existence of strong autofluorescence signals especially in the UV and visible parts of the spectrum. In addition, the short penetration of visible light restricts it to in vitro applications. New NIR fluorophores have been developed for the biological windows (BW). The first-BW (650- 950 nm) has been profusely studied although the penetration of light in this region is limited to a few millimeters. The second-BW (1000-1350 nm) is gaining interest because light penetration >1 cm can be obtained.[1] However, the existence of autofluorescence limits the useful wavelengths to the region from 1200-1350 nm, thus reducing the number of available probes for in vivo imaging. [2]

In this work, we present the elimination of autofluorescence signals in in vivo imaging, which takes advantage of the long luminescent lifetimes of trivalent rare earth ions (~100 µs) compared with the lifetime of the biomolecules causing this autofluorescence (<<1 ns). The combination of this with their emissions in the second biological window has allowed us to obtain deep tissue autofluorescence free images by using a simple time-gated set up.

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Nanoengineering properties through porous alumina

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The understanding of how the properties of the materials, such as thermal conductivity and electrical conductivity, can be tailored by growing nano-scale structures that affect them, is the main aim of this work. The fabrication of nanowires with diameters down to 12 nm and the recent development of three-dimensional nanostructured networks based on the controlled pulsed anodization of aluminum [1] open the possibility of tailoring the properties in a certain range.

A review of ways of tailoring different properties of materials through nanostructuration with the aid of porous alumina templates will be presented. For instance, in the case of the thermal conductivity, it has been demonstrated how this parameter can be experimentally changed and measured [2]. Moreover, the understanding of the reasons behind this change and how to control from a theoretical point of view has been also pursued. In the case of electrical conductivity, the effect of topological insulating appears in different materials when they are structured at the nano-scale [3].

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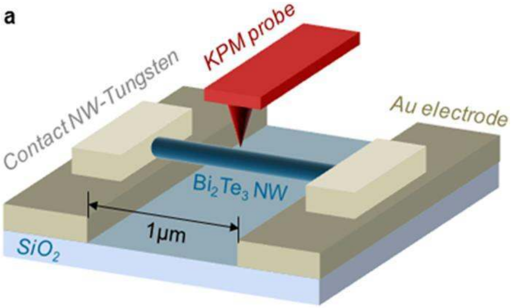

Figure 1: Measurement arrangement for the measurement of the electrical conductivity on the surface of a nanaowire [3]

Automated Graphene Transfer System for Graphene solar cells

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Although graphene grown by chemical vapor deposition (CVD) has proven to be an excellent material for electronic applications [1], an inconvenience of this method is the need of transferring the thin graphene layer from the initial metal catalyst to a suitable final substrate. A manual transfer method was developed in order to overcome this issue. It consists of protecting the graphene with a polymer layer, wet-etching the growth substrate, cleaning with deionized water and finally depositing the resulting polymer/graphene membrane onto the desired target substrate. Some drawbacks of this method are that it requires handling skills to perform it, that it is time consuming, and that it is not suitable for an industrial process. An optimized method based on a roll-to-roll system can overcome some of the manual method limitations, but it is mainly focused on flexible, transparent electrodes applications.

We report a lab-scale system designed to automatically transfer graphene to arbitrary substrates [2], but adapted it for industrial applications like solar cells. The system is composed of several modules that control the process temperature, the liquid flow and the overall system state. A microcontroller is used as the real-time control. The passive components of the system are depicted in Fig. 1. A PTFE tube encloses the graphene sample during the whole process. All this pieces are immersed in a liquid, starting with an etchant solution and changing gradually into deionized water for the final steps. Finally, graphene solar cells were processed using a manual method and our automatic method for comparison, showing higher mobilities and less charge impurities for the latter one.

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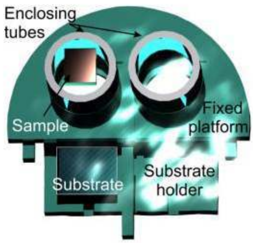

Figure 1: Graphene automated transfer system

Tuning of the photophysical properties of core-shell silica nanoparticles for bio-imaging and photodynamic therapy

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Abstract Spherical core-shell silica NPs with an external surface functionalized by amino groups and with an optimal average size around 50 nm, suitable for biomedical applications, have been successfully synthesized by a Stöber-modified method.[1] An optimization of the properties of fluorescent dye embedded in their core and of various photosensitizers (PS) grafted on the shell was carried out. By the encapsulation of fluorescent Rhodamines in the core at an optimal concentration to limit reabsorption, relatively high fluorescence quantum yields ($\phi_{fl} \geq 0.3$) were obtained, which allowed their tracking by fluorescence microscopy techniques and improved the time scale for detection due to the increase of dye photostability. A careful investigation of the stability of NPs suspensions showed a strong modification upon grafting of the PS. By covalent grafting of original lab-made halogenated 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) photosensitizers to the external shell of silica, good singlet oxygen quantum yields (Φ_Δ ~ 0.35-0.40) were obtained in ACN and chloroform solvents. Such quantum yields are globally much higher than those of similar NPs using grafted Rose Bengal (RB) as PS (Φ_Δ ~ 0.10-0.27). The resultant singlet oxygen quantum yields were related to the agglomeration of NPs, which depends both on the type of photosensitizer and on the amount of grafted PS. Finally, by the combination of two chromophores with overlapping absorption bands and complementary actions, namely a rhodamine with high fluorescence efficiency in the silica core and a BODIPY or RB with a high singlet oxygen quantum yield grafted on the shell, NPs with dual functionality were characterized (ϕ_{fl} ~ 0.10-0.20, Φ_Δ ~ 0.16-0.25), opening the route for theranostics (bioimaging and PDT).[2] Accordingly, by proper choice of the dyes, of their concentration inside and onto the NPs and of their grafting method, fine-tuning of singlet oxygen production and fluorescence emission is made possible. Further experiments will be soon carried out to improve the stability of the NP in polar solvents, and particularly in aqueous suspension, in order to be able to design "in vitro" phototoxicity experiments.

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Figures

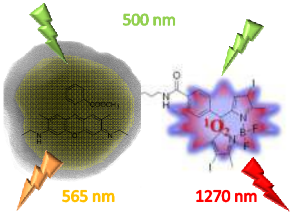

Figure 1: Schematic illustration of Silica nanoparticles with fluorescent Rhodamine embedded in the core and BODIPY photosensitizer grafted on the shell, generating fluorescence emission and singlet oxygen, respectively, under green excitation light

Pyrite surface pre-treatment drives molecular adsorption: cystine on pyrite(100) investigated by X-ray photoemission spectroscopy and low energy electron diffraction

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Abstract

We have demonstrated that the annealing process for cleaning pyrite surfaces is a critical parameter in promoting ordering on the surface and driving surface reactivity. Furthermore, we describe a spectroscopic surface characterization of the presence or absence of the surface ordering, as indicated by the Low Energy Electron Diffraction (LEED) pattern, as a function of the surface annealing process. Complementary X-ray photoemission spectroscopy (XPS) results provide evidence that longer annealing processes of over 3 hours repair the sulfur vacancies in the pyrite, making FeS species partially disappear in favor of FeS_2 species[1]. These features play an important role in molecular adsorption. We show that in the case of the cystine amino acid on the (100) pyrite surface, the substrate structure is responsible for the chemical adsorption form. The presence of an ordered structure on the surface, as indicated by the LEED pattern, favors the cystine NH_3^+ chemical form, whereas the absence of the surface ordering promotes cystine NH_2 adsorption due to the sulfur-deficient surface. The cystine molecule could then act by changing its chemical functionalities to compensate for the iron surface coordination. The chemical molecular adsorption form can be selected by the surface annealing conditions, implying that environmental[2] conditions could drive molecular adsorption on mineral surfaces. These findings are relevant in several surface processes, and they could play a possible role in prebiotic chemistry surface reactions and iron–sulfur scenarios[3].

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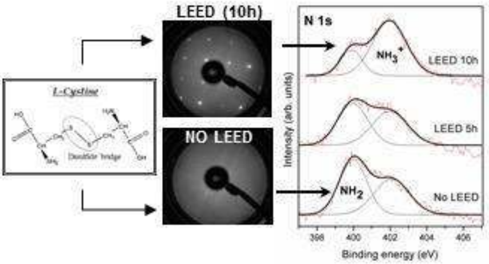

Figure 1: Annealing process for pre-treatment pyrite surfaces is a critical parameter in promoting ordering on the surface shows by LEED pattern and it has chemical implications on the cystine adsorbed molecules confirmed by XPS.

Development of new models and systems to micro- and nanoscale supported in high-precise functional replication of the clone instrumentation of MEMS and NEMS as products of the researches of the Nanotechnology Laboratory FOSUNAB

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Abstract.

This work shows a technology of artificial cloning for industrial sensors by means of the use of neural networks and genetic mapping. The neural networks allow develop to the intelligent structure of the micro- nanosensors, for it, the method of activation of random values is used to train the sensors and to carry out the learning starting from real devices, the genetic mapping allows the generation of codes for the cloning procedure, for it the mutation processes, crossing, reproduction and investment are used also, an example of a cloned sensor that determines the index of viscosity of lubricant oils with fenol for a monitoring system is briefly explained. The method include the application and interpretation of the genetic mapping that it contains; the codes of the functional structure of the sensor, the mapping is a group of bars of codes that describe the functional operative units of the micro- nanosensors, each operative unit is formed by unitary elements that represent a part of the operation of the sensors such as deviation of the angle of incidence, variation of the intensity of the sheaf of light, etc. A code is a series of digits that represent a part of the operation of the micro- nanosensors where each digit represents a position inside the functional structure (see Figure. 1). The cloned by functional replication the utilities are criteria likeness that apply measured a dimensional and they include parametrical characteristics of the real devices to clone that allow a micro- nanosensors to reach a cloned version.

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Figures

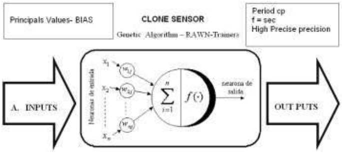

Figure 1: Neural network and genetic algorithm applied scheme for micro- nanosensors clone

Sheet and edge plasmonic modes in shaped graphene nanoresonators

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Plasmons in graphene nanoresonators have large application potential in photonics and optoelectronics, including tunable photodetectors, sensors, reflect-arrays or modulators. Their future efficient design will critically depend on the precise knowledge and control of the plasmonic modes. Particularly, highly confined edge modes have been predicted, which could benefit enhanced light-matter interactions and the performance of graphene-plasmonic devices. Here, we apply near-field nanoscopy (Fig. 1a) to analyze in real space, for the first time, plasmon modes in tailored disk and rectangular graphene nanoresonators at mid-infrared frequencies. The near-field images exhibit intriguing patterns and features (Fig. 1c), indicating the interference of manifold plasmon excitations. A simple model well reproduces the two-dimensional experimental patterns (Fig. 1d), allowing us for identifying edge and sheet modes, as well as for separating them either spatially or in energy. We also find that puzzling negative plasmonic image contrasts are governed by a spatially varying Fano-like interference between the near field of the probing tip and the graphene plasmons. We anticipate that real-space analysis of GPs could be of great benefit for the development and quality control of emerging graphene plasmonic technologies, particularly when novel design concepts and 2D material heterostructures have to be tested and verified. Further, we believe that the developed understanding of graphene-plasmonic near-field contrasts is broadly applicable to other 2D materials [1].

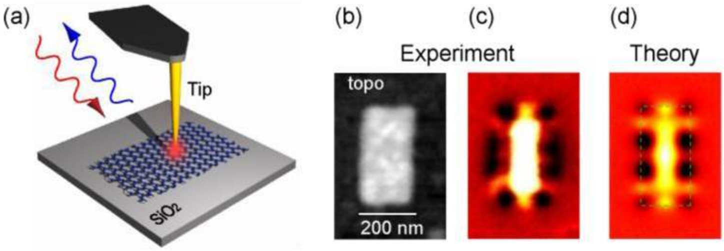

Figure 1: (a) The schematics of the concept of the experiment. A sharp metallic tip is illuminated by the external source. The strong near-field (hot spot) is created at the tip apex. The tip near-field apex excites the plasmons in the graphene rectangle. The tip is scanned above the rectangle and the scattered signal (proportional to the near-field of the plasmon) is recorded as a tip position. (b) Topography of the graphene rectangle. (c) Experimental near-field image of the graphene rectangle. (d) Simulation of the near-field image of the graphene rectangle.

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Hybrid magnetic and luminescent nanostructures for self-monitored photothermal therapy

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Superparamagnetic iron oxide nanoparticles (SPIONs) are of interest as contrast agents for magnetic resonance imaging (MRI) and for therapeutic applications due to their potential heat dissipation in alternating magnetic fields. Recently it was also demonstrated that they can be employed for photothermal therapy (PTT) due to their strong light absorption and efficient transformation of IR-radiation into heat.[1]

In this work, we were interested in studying the photothermal properties of SPIONs by measuring the light-to-heat conversion, while thereby also creating multifunctional magnetic nanostructures (MNS) for temperature-controlled localized photothermal therapy. Furthermore, we wanted to achieve both PTT and luminescence-based nanothermometry in the biological windows; regions in the IR in which tissue penetration and subcutaneous applications of light are possible. Towards this goal we encapsulated SPIONs jointly with LaF_3:Nd nanoparticles, which act due to the presence of the Nd-dopant as sensitive nanothermometer, allowing full control and monitoring of the localized heat generation.

The MNS we will present, were synthesized by encapsulation in PLGA, a biocompatible polymer suited for in vivo applications. The resulting NS were chemically and spectroscopically characterized and their applicability for subcutaneous PTT was demonstrated in ex vivo experiments, while their magnetic properties remained. Hence, the MNS open a door for in vivo controlled photothermal therapy.

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Synthesis of Fluorescent Nanovesicles Quatsomes for Bioimaging

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Nowaday, fluorescent organic nanoparticles (FONs) have become a very interesting tool for bioimaging. In particular dye-loaded small unilamellar vesicles (SUVs) permit the encapsulation of large quantity of fluorophores in a very small space, drastically improving the brightness many-fold compared to single organic dyes [1]. Their amphiphilic environment considerably stabilizes the poorly water soluble organic dyes in biological media permitting their use for *in vivo* and *in vitro* applications. In addition, considering the multifunctionality properties of nanoparticles, active delivery and site specific targeting could be developped raising real interest in the field of theranostic.

Here we presente new type of FONs based on the use of quatsomes [2], a new type of nanovesicles. Quatsomes are constituted from quaternary ammonium surfactants and sterols which self-assemble forming stable amphiphilic bimolecular building-blocks with the appropriate structural characteristics to form, in aqueous phases, closed bilayers. The outstanding thermodynamic stability of these nanovesicular architectures, the high vesicle to vesicle homogeneity in size, lamellarity and chemical composition, their stability upon dilution, their low toxicity, their good recovery after liophilization and the availability in pharmaceutical grade of their components, make them ideal colloidal nanoparticles for the engineering of a new class fluorescent probes, with optical, targeting and delivery properties easy tunable through self-assembly strategies. Three different strategies were used for the loading of molecular commercial and non-comercial dyes in quatsomes [3]:

i) The decoration of cationic quatsomes with anionic water-soluble dyes,
ii) The partial substitution of cholesterol with a dye-functionalized cholesterol,
iii) The encapsulation of hydrophobic dyes inside the bilayer via a *membrane anchoring* mechanism.

In particular, this last strategy considerably improved the water dispersibility of hydrophobic dyes containing long alkyl chains by their ability to penetrate the membrane bilayer of quatsomes. When prepared using compressed fluids methodology (DELOS-SUSP) [4], these fluorescent vesicles were stable over months and demonstrated high brightness. In some cases, dyes loaded in quatsomes demonstrated better photostability than single dye in solution.

Therefore, quatsomes constitute a interesting platform for the nanostructuration of organic dyes in water, preserving their optical properties while being highly versatile. These finding open a huge range of possibilities in their use for diagnosis and theranostic applications.

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Electrochemical Bioassays Based on Modulated Growth of Quantum Dots

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We pioneered bioassays in which analytes modulate the formation of CdS quantum dots (QDs) *in situ.* Our early assays were applied to fluorogenic determination of enzymatic activities of enzymes such as acetylcholine esterase[1], horseradish peroxidase[2], glucose oxidase[3] etc. We report a new class of sensitive electrochemical assays employing generation *in situ* of QDs suitable for determination of analytes using affinity interaction and oxidative properties of metal cations. In our new immunno assay alkaline phosphatase conjugated to antibody calalyzes formation of CdS QDs[4]. Irradiation of QDs with the standard laboratory UV-illuminator results in photooxidationof 1-thioglycerol (TG) mediated by Os–PVP complex on the surface of graphite electrode at appliedpotential of 0.31 V vs. Ag/AgCl. (Figure 1). We, also, designed a new assay based on microbead linked enzymatic generation of CdS QDs (Microbead QD-ELISA)[5]. The resulting QDs were detected by fluorescence spectroscopy, microscopy, and square-wave voltammetry (Figure 2). We discovered that cysteine (CSH) readily stabilizes CdS QDs growing in aqueous solutions. Oxidation of CSH by hydrogen peroxide (H_2O_2) at room temperature yields cystine (CSSC) which does not stabilize CdS QDs so efficiently as CSH does. Such oxidation causes the decrease in the rate of the formation of CSH-capped CdS. For the first time, we combined the oxidation of CSH with copper ions or biocatalytic oxidation of D-glucose catalyzed by glucose oxidase[6] (Figure 3). Electrochemical detection strategies employing semiconductor growth of CdS quantum dots (QDs) *in situ* open up new opportunities for highly sensitive detection of biological targets.

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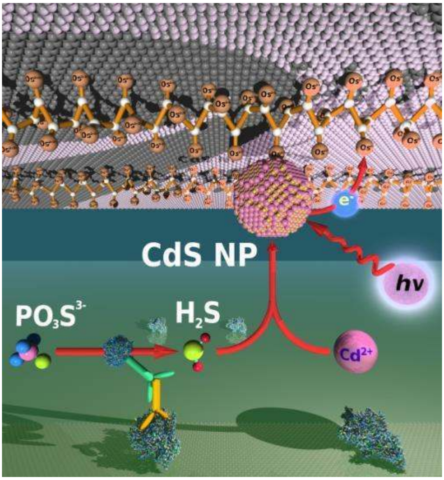
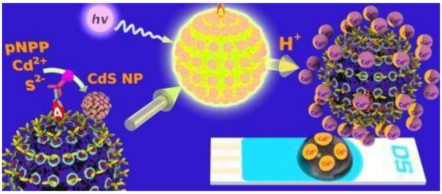
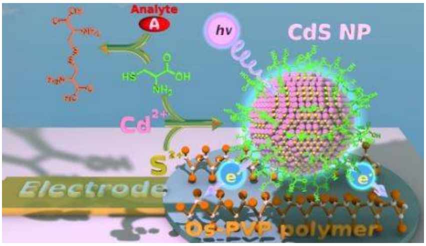
Figures



↑ **Figure 1:** Immunoassay using photoelectrochemical detection of enzymatically generated CdS QDs



↑ **Figure 2:** Microbead ELISA using biocatalytic formation of QDs for ultra high sensitive electrochemical detection



↑ **Figure 3:** Photoelectrochemical assay for copper and glucose using modulation of growth of Cysteine-capped QDs

Spin-Orbit driven effects in graphene based perpendicular magnetic anisotropy structures

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The development of all-graphene spintronic devices requires that, in addition to its passive capability to transmit spins over long distances, other active properties are incorporated to graphene. The generation of long range magnetic order and spin filtering in graphene have been recently achieved by molecular functionalization [1,2] as well as by the introduction of giant spin-orbit coupling (SOC) in the electronic bands of graphene [3]. We have incorporated these developments by designing novel perpendicular magnetic anisotropy (PMA) nanoarchitectures with tailored SOC in graphene and large chiral exchange interaction, commonly known as Dzyaloshinskii–Moriya interaction (DMI).

To do so, we have grown in ultra-high-vacuum (UHV) condition epitaxial multilayers with asymmetric interfaces on commercially availbale oxide single crystals (MgO). We were able to tune the PMA (K_U) and the DMI, in NM1/FM/NM2 structures, where FM is ferromagnetic Co layer, sandwiched between a NM1 non-magnetic metal and NM2 graphene (gr) sheet. We demonstrate strong PMA in such epitaxial systems with up to 20 MLs Co. We have characterized in-situ the electronics, chemical and magneto-transport properties of the samples by surface sensitive analysis, like X-ray absorption spectroscopy, LEED, as well as XAS-XMCD synchrotron based measurements. In addition, we have investigated the magnetic properties of the systems ex-situ by magneto-optical Kerr effect (MOKE), proving a strong PMA anisotropy for structures with up to 20 ML Co layer underneath gr [4,5].

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Mapping commensurability orbits in graphene antidot lattices

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Recent advances in the fabrication of high quality nanostructured graphene samples have enabled the investigation of mesoscopic phenomena requiring long range ballistic behaviour. An excellent example of this is the demonstration of multiple highly-pronounced commensurability peaks in the magnetotransport response of graphene antidot lattices encapsulated in hexagonal Boron Nitride[1].
Such peaks are predicted to occur when the cyclotron radius is tuned to match important length scales in the system, so that electrons are pinned in orbits around single or groups of antidots or skip regularly between neighbouring antidots.
In this work[2], we demonstrate that the experimental magnetotransport measurements are captured with remarkable accuracy by a fully quantum-mechanical multiprobe transport simulation. Furthermore, by mapping local current behaviour, we explicitly associate specific commensurability peaks with different electron trajectory types and explore their dependence on the antidot geometry. Finally, by tuning the Fermi wavelength we can move between the semiclassical and quantum regimes and demonstrate the suppression of commensurability effects.

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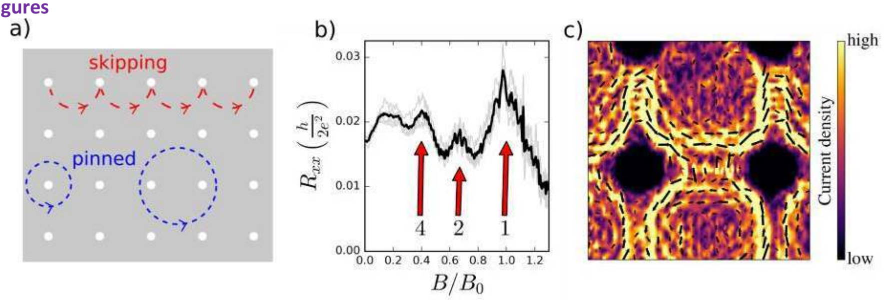

Figure 1: a) Schematic illustration of pinned and skipping orbits in an antidot lattice. b) Simulated commensurability peaks in the longitudinal resistance of a graphene antidot lattice Hall bar device. Red arrows highlight the expected positions for pinned orbits around 1, 2 or 4 antidots. c) Local current behaviour in the device at the principal ('1') commensurability peak – skipping orbits between neighbouring antidots are clearly visible.

Wavelength-scale patterning of colloidal quantum-dot assemblies: a building-block approach to integrated photonics.

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Colloidal quantum-dots (cQDs), or semiconductor nanocrystals, are highly versatile building blocks that combine size-tunable optical properties with low-cost wet-chemical methods. High quantum yields (>90%) and spectrally narrow emission throughout the visible and near-infrared range have placed cQDs among the highest color-quality emitters available.[1,2] As such, they are ideal candidates for the bottom-up construction of photonic devices, where the combined tunability of the nanoscale building-block and the wavelength-scale photonic structure introduces new levels of control over optical effects.

Here, we present a methodology to produce such patterned colloidal assemblies using template stripping.[2] Mechanical cleaving (i.e. "stripping") of a cQD film from a patterned hard silicon template allows for high-fidelity transfer of almost arbitrary shapes, yielding high resolution (<100 nm) and wafer-scale photonic structuring of cQD films. Using this technique, we are able to construct fully functioning photonic components composed purely out of cQDs. Examples include low-loss waveguides, high quality-factor ring-resonators, and distributed feedback lasers with heavily reduced thresholds. Moreover, we will demonstrate how synthetic control over the cQD building block can enhance the performance of these photonic devices, for example through wavelength tuning and core-shell based Stokes-shift engineering.

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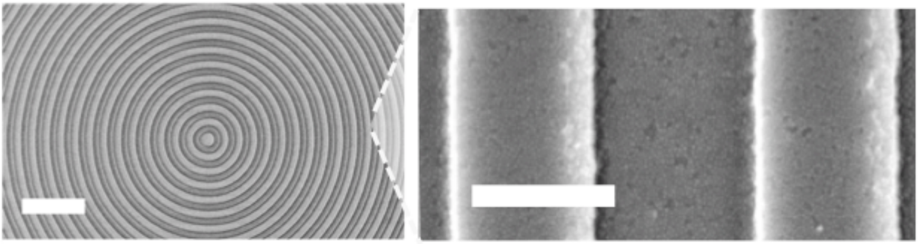

Figure 1: Structural detail of a distributed feedback laser composed purely out of colloidal quantum dots (~10 nm in size). Scale bars are 2 µm and 200 nm.

Plasmonic Heaters Monitored in-situ with Nd^{3+}-based Nanothermometers as Candidates for Photodynamic Therapy in the Near-Infrared

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The development and even the survival of cells and bacteria only happen in a narrow range of temperatures. Accordingly, a controlled and localized temperature increase can be exploited as a therapeutic tool for infections or cancer. With this idea in mind, plasmonic nanostructures have been proposed as efficient nanoheaters that can be activated with light.[1, 2] However, for the treatment to be efficient and to minimize the chances of overdosing, it is needed to monitor the actual temperature of the treated area. Since temperature measurement at the nanoscale is also relevant in order to study additional biological processes related with the metabolism of cells, over the last years several molecules or nanomaterials with thermally-dependant properties have been developed as thermal probes.[3] In this work we have developed inorganic nanoparticles doped with Nd^{3+} that can be used as optical probes of temperature. These nanoparticles have been combined with gold nanostructures in order to study their heating efficiency and thermal stability. As *in vivo* applications would benefit from high penetration depths of the probe signal and the excitation, both the heater and the thermometer have been designed to work at wavelengths within the biological transparency windows.

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Synthesis of Janus Magneto-Plasmonic nanoparticles. Multimodal imaging and SERS detection

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Multicomponent nanoparticles have attracted strong interest in the last years due to the unique combination of properties present at the nanoscale that make them suitable for a high set of applications. Among them, Janus nanoparticles, characterized by two different surface regions, can be of great interest to produce a specific interaction with interfaces, biomolecules, membranes etc.

Here, we report the synthesis of Janus nanoparticles composed of Au-Fe_3O_4 nanostar-nanosphere (also called nano-octopueses) through two consecutive seed-mediated-growth steps. Electron tomography combining HAADF-STEM and EDX was performed to evaluate the Janus character of the nanoparticles (figure a-e). The nanoparticles showed superparamagnetic properties and a high plasmonic absorption at the near-IR (figure f).The extraordinary versatility of these nanoparticles has been tested in analytical sensing using Surface-enhanced Raman spectroscopy (SERS), and multimodal imaging. The resulting experiments showed the high Raman enhancement of these nanoparticles thanks to the Au nanostar part of the Janus nanoparticles that can be further amplified with the use of magnetic concentration, allowing nanomolar detection in very small sample volumes. Furthermore, with the use of combined gold and iron oxide in a Janus configuration we demonstrate how these magnetoplasmonic nanoparticles act as superior contrast agents in a high variety of imaging techniques, including cell imaging in dark and bright field, multiplexed SERS mapping and 3D tomography in magnetic resonance imaging (MRI) and computed tomograpy (CT) among others.

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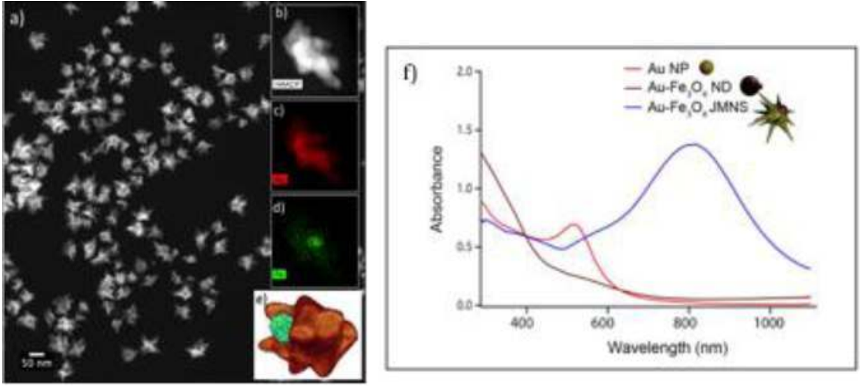

Figure 1: a-e) HAADF-STEM, EDX mapping and combined electron tomography. f) UV-VIS of the Janus nanostars and the initial seeds used in the synthesis.

Hyperthermia produced by magnetic nanoparticles as an alternative method to control a major foodborne pathogen

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Salmonella enterica is responsible for the majority of the reported foodborne outbreaks, and that is why it is considered one of the most important foodborne pathogens nowadays [1]. Like many others bacteria, *S. enterica* can survive disinfection and resist a wide variety of biocidal agents [2]. Nowadays, the synthesis of superparamagnetic nanoparticles (MNPs) and its application in magnetic hyperthermia (MH) is of great interest, with MH being recently reported as a viable alternative to traditional disinfection methods against bacteria [3]. However, fundamental studies comprising the MH effect on different populations of planktonic cells and biofilm cells are scarce. Therefore, this work aimed at evaluating the effect of MH on different populations of planktonic cells and biofilms of *S. enterica*.

The work was performed using a *S. enterica* collection strain (NCTC 13349), which different planktonic cell populations (lag, exponential, and stacionary phase) were adjusted to a final concentration of $\approx 1 \times 10^8$ cells/ml, while biofilms were formed in silicone coupons. Samples containing both magnetite nanoparticles and *S. enterica* cells or biofilms have been subjected to an alternating magnetic field of chosen amplitude 100 Oe with frequency of 873 kHz until different temperatures were reached. In order to evaluate the bactericidal effect of MH, survival of planktonic and biofilm cells was determined by colony forming unit (CFU) enumeration. Based on the most relevant results, cell membrane integrity and the effects of MH on cells surface and biofilm structure were analysed through microscopy techniques.

Results showed that the high structural-magnetic quality magnetite nanoparticles used were effective against all planktonic cell populations and biofilms under an oscillating magnetic field. In fact, MNPs-based hyperthermia was able to promote a significant cell viability reduction on all planktonic cell populations both bacterial lyfe styles. Nonetheless, planktonic cells were more tolerant to MH than biofilms, possibly due to diffusion limitations along these bacterial communities. Microscopy images of planktonic cells and biofilms showed that MH can affect cell membrane integrity as well as the biofilms' structure.

In conclusion, this work presents evidences of the bactericidal effect of MH produced by MNPs against *S. enterica*, both regarding planktonic populations and biofilms. This ability of MH to control a major foodborne pathogen constitutes a novel contribution to the finding of new useful applications of hyperthermia.

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Fermi Level Pinning and Orbital Polarization Effects in Molecular Junctions

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Self-assembled monolayers (SAMs) provide a convenient way for tuning the work function of electrodes and controlling the hole or electron injection barriers.[1] Besides, SAMs have also promising applications in molecular electronics, where they act as a linker between two electrodes. In molecular junctions, the electronic structure of the SAM/metal interface plays a dominant role on the final electronic transport properties that do not simply reflect the properties of the molecules. The key parameters are the alignment of the SAM conducting states relative to the metal Fermi level (E_F), and the interplay between the interfacial and intramolecular electronic couplings.

Recent theoretical studies have suggested that the frontier molecular orbitals can be pinned to the Fermi level (implying that the changes in the HOMO level energy of a conjugated core upon electroactive substitution in the gas phase is not recovered in the junctions) and electronic polarized under the application of a bias.[2] To further shed light on these two phenomena, we investigate here the electronic structure of a series of organic conjugated wires varying by the nature of the central ring when deposited on Au (111) using Density Functional Theory (DFT) calculations, with a special emphasis given to the variations of the work function of the metal. We also use a Non-Equilibrium Green´s function formalism coupled to a DFT framework to simulate the I/V curves of single-molecular junctions and to rationalize them from the evolution of the transmission spectra under bias.

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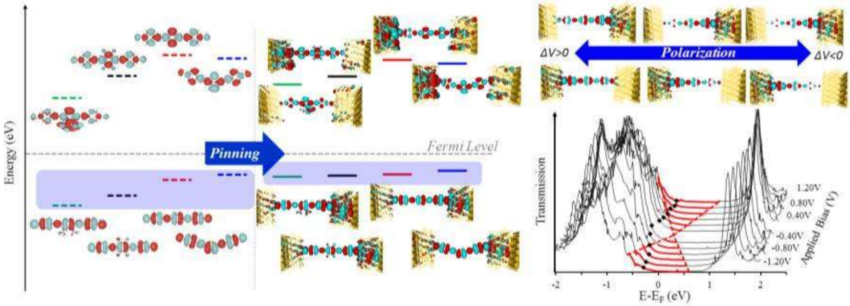

Figure 1: Schematic representation of Pinning and Polarization Effects in Molecular Junctions at equilibrium and under biases.

New Standards in 3D Micro Printing

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The technique of two-photon polymerization (TPP) is a powerful 3D printing solution for miniaturization which offers sub-micrometer features sizes and resolution, design freedom beyond conventional micro/nanolithography and short iteration design cycles. Here, we present how 3D micro printing works and we further discuss both scientific disruptive breakthroughs and applications in industry in a wide range of fields spanning from photonics and plasmonics to microfluidics and biomedical devices.

While TPP was previously known for ultra-fine yet small objects mostly viewed under the scanning electron microscope, now mm^3-scale fabrication (Fig. 1, left) has become the novel standard in 3D microfabrication with still sub-micrometer precision. Application examples in optics and photonics include photonic crystals, metamaterials [1, 2], optical cloaks [3], diffractive optical patterns (Fig. 1, center), photonic multi-chip integration [4] and high-precision free-form micro-optics [5]. Furthermore, gears, mixers, micro-robots [6] and micro-needles for painless drug delivery, high aspect ratio micro pumps (Fig. 1, right) and 3D scaffolds for cell culture [7] will be discussed.

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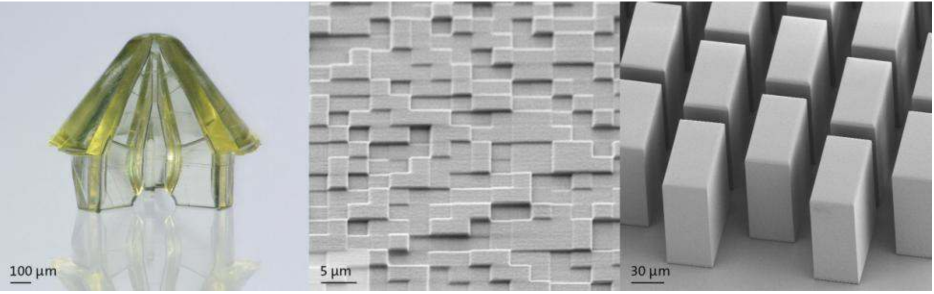

Figure 1: (from left to right) 3D printed nozzle. Diffraction multilevel pattern. High aspect ratio microfluidic capillary pump.

Highly ordered honeycomb polystyrene patterns decorated with polyoxometalates for catalytic applications

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Breath figure process is a cost-effective method for preparing highly ordered honeycomb patterns from polymer solutions. In this process, a polymer solution is casted onto a substrate under adequate humidity and the evaporation of the solvent cools down the solvent/air interface inducing the condensation of small water droplets.[1] The variation of the concentration, solvent and relative humidity enables the control over the formation of honeycomb patterns.[2] The fabrication of honeycomb arrays has received an increasing interest due to the potential applications of these structures in different areas, such as tissue-engineering, membranes, or catalysis.[3] In our study, honeycomb patterns have been obtained from polystyrene/poly(polystyrene-*b*-polyacrylic acid) blends. The resulting porous arrays have been decorated with polyoxometalates in order to obtain polymer films with maximized catalytic capability.

Polyoxometalates are anionic transition metal-oxo clusters of nanometric size that can act as both strong Brønsted acids and oxidation catalysts showing fast and reversible multistep redox processes without significant structural changes. The decavanadate-based $[Cu(cyclam)][\{Cu(cyclam)\}_2(V_{10}O_{28})]\cdot 10H_2O$ microporous hybrid (cyclam = 1,4,8,11-tetraazacyclotetradecane) has been recently employed as catalyst for the oxidation of the highly stable, tricyclic alkane adamantane.[4] A scheme of the functional polymeric surface decorated with the Cu(cyclam)-decavanadate hybrid is shown in Figure 1.

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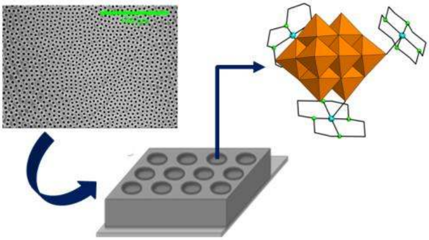

Figure 1: Poly(styrene)/Poly(styrene-*b*-acrylic acid) blend breath figures decorated with $\{Cu(cyclam)\}^{2+}$ and $(V_{10}O_{28})^{6-}$·units.

Rational design of supramolecular devices

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In this talk I will describe how a combination of multi-scale computer models, nanoscale materials characterisation and macroscopic electrical device measurements has bred a new class of high-performing, long-lived molecular devices that are approaching the performance of CMOS electronics but which are based on monolayers of redox-active molecules trapped between conductive electrodes. I will show how judicious choice of molecule length, headgroup, electrode material and electrode quality (Fig. 1) has a large impact on device performance that can be rationalised using molecular models [1] that in turn provide a virtual sandbox for the rational design of junctions with pre-programmed functionalities for a broad range of applications in nanoelectronics as well as plasmonics and nanomedicine.

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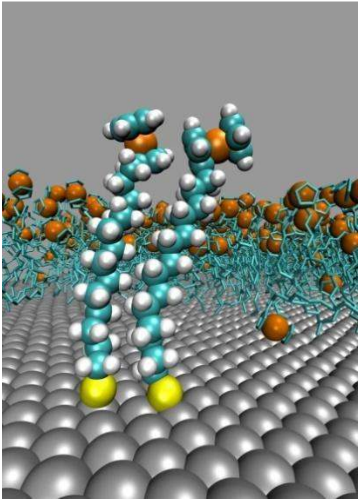

Figure 1: Ferrocene-alkanethiolate self-assembled monolayers (SAMs) on silver electrodes provide robust high-performance molecular rectifiers.

Polyurethane foam/graphene nanocomposites

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INTRODUCTION

Graphene is a 2D material comprised of carbon atoms forming hexagonal lattices. Its characteristic structure confers graphene excellent electrical, thermal, mechanical and optical properties, becoming an interesting nanomaterial for its application in polymer nanocomposites. Graphene was obtained by liquid exfoliation from graphite and size selected by centrifugation[1]. The obtained graphene was used to confer electrical conductivity to polyurethane foams incorporating graphene by impregnation technique.

METHODS

Graphene was obtained by liquid exfoliation of graphite powder by sonication with N-methyl-2-pyrrolidone (NMP). The resulting dispersion was centrifuged at different rates to obtain fractions of different sizes of graphene. Solid graphene was isolated by filtration obtaining also recoverable NMP. Morphology of graphene was analyzed by Raman spectroscopy, atomic force microscopy (AFM) and transmission electron microscopy (TEM) and electrical properties were assessed by electrostatic force microscopy (EFM) technique.

For the preparation of polyurethane foam nanocomposites, a dispersion of graphene in cyclohexane at 1 mg mL^{-1} was prepared. Foams were immersed in the graphene suspension and were sonicated for different times. Microstructure and properties of nanocomposites were analyzed by thermogravimetric analysis (TGA), scanning electron microscopy (SEM) and the assessment of electrical properties.

RESULTS

Raman spectra of graphite and graphene fractions showed typical bands associated with carbon materials. Differences on flake size of graphene are evidenced by the ratio of I_D/I_G Raman bands intensity since it is related with edge defects[2]. According to AFM analysis, flake sizes change in 5-0.4 µm range and flake thicknesses in 8-1.5 nm range when final centrifugation rate is changed from 500 to 4000 rpm, respectively. The low layer content of graphene fraction centrifuged at the highest rate was verified by TEM analysis and their conductive properties were confirmed by EFM analysis.

By using the ultrasound assisted impregnation method graphene flakes were adhered to polyurethane foam matrix. The presence of graphene flakes was confirmed by SEM analysis. The adhered graphene content on the surface was calculated from TGA results and varied with the sonication time. Graphene provides foam matrix with electrical conductivity. Graphene content has high influence of electrical resistance values. Apart from this, it was seen that the electrical resistance of the nanocomposites was sensitive to compressive mechanical deformation, diminishing with the elastic bending of cell struts and the contact posterior to cell collapse3.

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Improvement of the Enzymatic Activity of α-Galactosidase Using Nanovesicles with application to Fabry Disease treatment

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Fabry disease is, among the lysosomal storage disorders, a rare inherited disease caused by loss of function of the enzyme α-Galactosidase A (GLA) [1]. One of the commercially available treatments is based on the intravenous administration of GLA. This enzyme replacement therapy (ERT) demonstrated positive short-term effect reducing the progression of the disease and improving the quality of life in patients. However, ERT exhibits drawbacks such as the degradation of the exogenously administered enzyme, its limited efficacy in patients with an advance stage of the disease and the extremely high cost of the treatment.

In order to improve the delivery efficacy and the systemic circulation of the current treatment, nanovesicles containing GLA were prepared as novel drug delivery systems (DDS). The incorporation of GLA in nanovesicles was obtained following the DELOS-SUSP methodology, based on the use of compressed CO_2 (**Figure 1, left**) [2]. Moreover, a c(RGDfK) peptide ligand was incorporated in the membrane bilayer of the vesicles to enhance the targeting and the uptake efficiency of the GLA-loaded conjugates to the affected cells. The latter constitutes a major challenge in the treatment of lysosomal storage disorders.

Here, the preparation of different nanovesicles and comparative results obtained with the GLA-loaded conjugates and the free GLA enzyme will be presented [3]. Importantly, *in vitro* efficacy studies in GLA deficient cells of Fabry KO mice showed that the GLA-nanoformulations were able to reduce lysosomal Gb3 deposits more efficiently than the free enzyme (**Figure 1, right**), in agreement with a greater specific activity also encountered. This finding indicates that (i) such multifunctional nanovesicles are uptaken by GLA deficient cells, (ii) the GLA-nanovesicles reach the lysosomal compartment, and (iii) the cargo (GLA) is efficiently released so that the GLA activity in the cells is restored. Thus, the remarkable results obtained here prove the great potential of DELOS-SUSP method for the production of new nanomedicine candidates based on enzyme-nanovesicle conjugates. The development of these new GLA-nanoconjugates up to the end of the regulatory preclinical phase will be carried out under the frame of the European Smart-4-Fabry project (H2020-NMBP-2016-2017 GA 720942).

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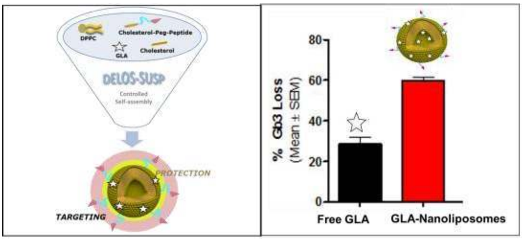

Figure 1: Nano-GLA multifunctional nanoformulation, manufactured by the DELOS-SUSP platform (left). Effect of free GLA and GLA-Nanoliposomes in the reduction of Gb3 deposits in aortic endothelial cells of Fabry KO mice (right). Represented values correspond to mean ± SEM value.

Physicochemical and Optical Properties of Mesoporous Anodic Alumina Particles and Their Use in Biotechnology

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Nanometric and micrometric particles have recently been used for the development of a wide range of applications, being biotechnology the area with the greatest social impact nowadays. Particles that respond to variables in specific tissues in the human body are a novel and promising strategy in health care and quality of life. Excellent results have been obtained in recent studies with particles in the micrometric and nanometric size range in vitro and in vivo [1].

Mesoporous anodic alumina (MAA) is a nanostructured material, excellent for developing porous particles. It is characterized by hexagonally-ordered straight nanometric pores that provide an exceptionally large effective surface area (hundreds of m^2/cm^3) [2]. Its porous morphology (pore size, interpore distance, porosity, and thickness) can be molded by the anodization conditions (voltage and time of anodization, temperature, and acid used as electrolyte), with a cost-effective and precise control fabrication [3]. Moreover, the surface of MAA can be chemically modified with organic compounds [1] and its compatibility with biological tissues has been demonstrated with its use in orthopedic prosthetics, dental and coronary stents, cell culture scaffolds, and immunoisolation devices [4].

MAA particles with a porous surface and porous body present large effective surface area and large pore volumes, which make them excellent candidates for drug delivery systems and sensing [5]. Another singular characteristic that distinguishes MAA particles from particles made of other materials is their inherent photoluminescence in the visible spectrum range (Figure 1).

In this work, we present different MAA particles with a micrometric and nanometric size and we study and evaluate their physical, chemical and optical properties for a wide range of applications in the biomedical and biotechnological fields

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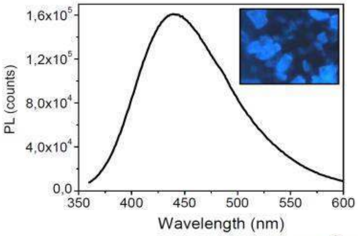

Figure 1: Photoluminescence of MAA particles (excitation wavelength 340 nm). Inset: Blue fluorescence field image of MAA particles

Oral Contributions
Parallel Sessions

Near-field imaging of resonating hyperbolic polaritons in nanorod antennas made of boron nitride

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The properties of polaritons in layered materials, such as van der Waals (vdW) materials, differ fundamentally from that of polaritons in conventional isotropic materials. Due to the layered structure of the materials, polaritons present hyperbolic dispersion, enabling unusual optical phenomena such as subdiffraction imaging and spontaneous emission engineering. Here, we present the first near-field study of Fabry-Perot resonances in linear antennas made of a hyperbolic material. Specifically, we study hyperbolic phonon polaritons in rectangular waveguide antennas made of hexagonal boron nitride (h-BN) [1,2].

Through nanoimaging and spectroscopy experiments we reveal spectrally sharp resonances, exhibiting atypical modal near-field patterns that have no analogue in conventional linear antennas, such as the puzzling near-field oscillations across the h-BN rods as observed in Fig. 1. We will discuss a detailed experimental and theoretical analysis of the sharp resonances and near-field patterns, showing that the oscillations can be attributed to a single waveguide mode resonating along the longitudinal axis of the antenna. We will also discuss its physical origin.

Our work establishes a solid experimental and theoretical basis for the understanding of propagating and resonating hyperbolic polaritons in waveguides, which could lead to the development of novel, ultra-compact photonic devices [3].

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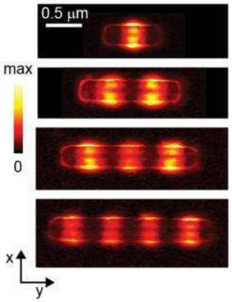

Figure 1: s-SNOM images of a set of linear h-BN antennas of different length L. Imaging frequency ω = 1432 cm-1. The nominal width and thickness of each antenna is 230 nm and 64 nm , respectively. From top to bottom, L= 746 nm, L= 1327 nm, L= 1713 nm and L= 2210 nm.

Nanoplasmonics from large-scale *ab initio* calculations: opposite trends in Ag and Na clusters

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An accurate description of electronic excitations is indispensable for understanding material properties and designing nanoscale devices. For instance, using large-scale TDDFT calculations, we have recently demonstrated the importance of taking into account the details of the atomic-scale structure [1] and the quantization of electron transport [2] in metal nanostructures in order to accurately describe their plasmonic properties. In this contribution we will compare the surface plasmon resonance of sodium and silver clusters within the same framework of iterative TDDFT [3]. Recent progress in our implementation made it possible to perform calculations of large clusters of diameters ranging from a few Å to 4–5 nm (Figure 1), counting up to 5000 silver atoms and using only modest computational resources (a 32-core node with 500GB RAM). With these new capabilities, we have characterized the size-scaling of the SPR frequency for both sodium and silver clusters. As expected these two materials show opposite behaviors that can be related to the different spill out of charge at the surface and to the additional screening created by the 4d electrons in silver.

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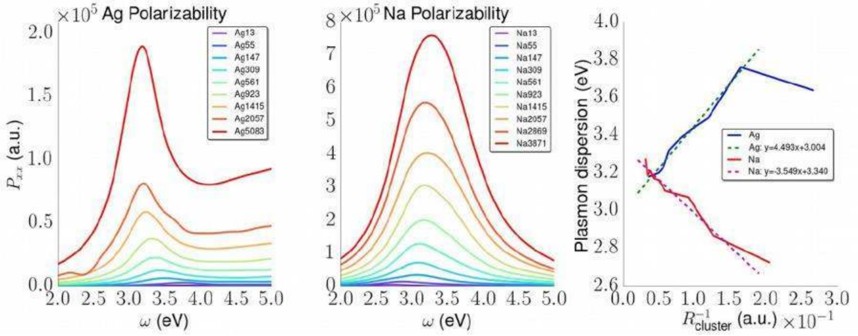

Figure 1: First and second column: optical polarizability for icosahedral silver and sodium clusters of different sizes. Third column: plasmon dispersion for silver and sodium cluster from abinitio calculations, the dashed lines show the linear interpolations.

High Refractive Index dieletric dimer as element unit for switching devices

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Low loss high refractive index (LLHRI) dielectric particles (like Si, Ge and other semiconductor compounds in the NIR) and smaller than the incident wavelength, have recently shown to be an alternative to the conventional metallic particles to overcome their inherent ohmic losses[1]. Furthermore, the coherence effects between the electric and magnetic excited resonances lead to interesting directionality properties[2,3] which, suitably handled, make them useful in many different applications for new designs of metamaterials, sensors or optical devices[4-6]. Here, we investigate both numerically and experimentally, the possibility of using a dimer of spherical particles made of LLHRI material, as elementary unit for building a binary switching device. This binary state will depend on the polarization of the incident radiation[7]. The study of this effect was done through the analysis of the linear polarization degree of the light scattered perpendicular to the exciting incident beam, $P_L(90°)$. This parameter contains information about the magnetic or electric character of the resonances. The scattered intensity at 90° reaches null or maximum values at the same frequency of the incident electromagnetic radiation perpendicular, I_S, or parallel, I_P, to the scattering plane, respectively. This effect is especially relevant when both particles are close enough and interact electromagnetically, as it is evidenced in Fig. 1.

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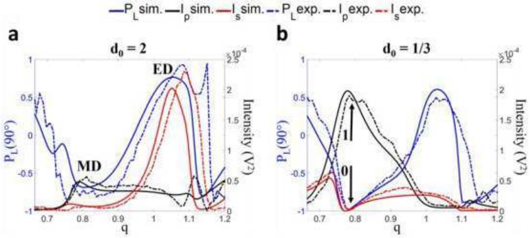

Figure 1: Linear polarization degree at the right scattering configuration and scattered intensities, I_P or I_S parallel and perpendicular respectively to the scattering plane, for a dimer of spherical silicon particles for two different distances between the particles as a function of the parameter size q ($q = 2\pi R/\lambda$ where R is the particle radius and λ is the wavelength of the incident radiation). In **a)** the relative distance between the particles is d_0 =2 (weak electromagnetic interaction) and in **b)** d_0 = 1/3 (strong electromagnetic interaction). d_0 is defined as the ratio between the dimer gap distance and the particle radius, R. Simulated (solid blue line) and measured (dashed blue line) $P_L(90^o)$. Simulated (solid red line) and measured (dashed red line) I_S. Simulated (solid black line) and measured (dashed black line) I_P.

Optical nanoimmunosensor based on periodic array of resonant nanopillars for real time detection of Okadaic Acid

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The field of optical sensors is continuously evolving towards the search of new transducers. Recently, a new transducer based on periodic array of resonant nanopillars (RNP) has been described [1,2]. Particularly, RNP composed by two Bragg reflectors (SiO_2/Si_3N_4) and a central cavity of SiO_2 have shown very interesting results, being suitable for label-free molecule detection [3] and also for real-time monitoring by using a common spectrophotometer [4].

Here we present the detection of okadaic acid (OA) -a toxin produced by several species of marine dinoflagellates and responsible of the syndrome known as diarrheic shellfish poisoning – by using a RNP biosensing system based on monoclonal antibodies (Ab), in a competitive working format. The surface is biofunctionalized with an OA competitor (BSA-OA), for the subsequent binding with the antibody, which signal is inhibited by the presence of OA. The label-free and real-time signal is monitored by using a microfluidic cell and a spectrophotometer.

Employing laser interference lithography, we fabricated RNP of different pitches and heights [5] and most sensitive nanopattern was selected to develop the biosensor. By using an IgG-antiIgG model, several biofunctionalization strategies were evaluated: activation and silanization processes were assessed to achieve covalently and stable immobilization of bioreceptor on transducer. Besides RNP real time response, the biofunctionalization was tracked by scanning electron microscopy (SEM).

Optimized functionalization protocol was applied for detection of OA. After immobilization of BSA-OA, we measured optical changes upon flowing solutions with different OA concentrations and calibration curve was evaluated. Smooth regeneration of antibody-antigen interaction allows reusing the surface for measuring several samples. Results show an OA limit of detection close to 5 ppb revealing the sensitivity of RNP assay as well as its rapidity (25 min/sample). These features constitute our OA sensor as a competitive analytical tool, since usually OA is determined by more complex and expensive techniques as HPLC.

This biosensing technology will be part of the Chemical Detection Unit of FP7 Enviguard project whose aim is the development of a biosensor device for real time and in-situ mesurement of chemical pollutants and biohazards (viruses, microorganism and toxins) to be used as an early warning system in acquaculture.

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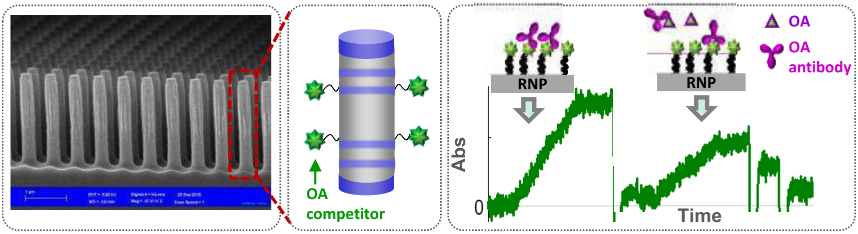

Figure 1: SEM image of RNP; biofunctionalized RNP; real time detection of OA (competitive assay).

Modelling emergent effects in low coordination geometries during metallic nanojunction formation

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Quantum phenomena that are not observed in bulk metals, but which manifest in low coordination geometries such as few-atom contacts [1, 2], suspended monatomic wires [3, 4] and free surfaces [5-7] are modelled by means of a combination of classical and quantum mechanical atomistic simulations; including, classical molecular dynamics, tight binding models and density functional theory. The roles played by the parent crystal structure and local electronic structure of the metal atoms in these low coordination environments are explored. Since emergent quantum properties, such as enhanced magnetism along suspended monoatomic wires [4], also directly affect the local geometry and electronic structure of the nanocontacts, a more accurate theoretical description is needed to resolve discrepancies between existing theoretical results and experiment. Additionally, such a description should lead to more informed predictions about metallic nanocontacts created from body-centered metal samples, which have not been the object of many studies thus far. In this work, we study the formation and rupture of gold, copper and tungsten nanocontacts, with the view of extracting trends that can be extrapolated to other transition metals, which are also frequently employed in the experiments, including platinum, iron, and silver.

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Optical Chirality in the Stacked 3D Ring-Split Ring Nanostructure

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Nanaostructures with plasmon enhanced chiral properties have drawn intense interest in the last years due to the potential applications in the detection and even asymmetric synthesis and catalysis of chiral molecules [1]. In the current work we propose experimentally a novel 3-dimensional (3D) nanostructure based on the stacked ring-split ring with an additional dot on top (Figure 1) [2], which performs a sound optical chiral effect in the wavelength range from visible to near infrared.
Hole-mask colloidal ligthography (HCL) method is chosen to realize the considered nanostructures over cm^2 [3]. Meanwhile, the top dot can be easily located along the perimeter of the structure (left in Figure 1), which actually controls the chirality and handness of the nanostructure. Furthermore, with this method it is possible to insert a ferromagnetic Co dot below the gap, which makes it possible to explore the intertwined magneto-optical and chiral effects or to control the chiral property with magnetic field [4]. Representative AFM images of two structures with complementary handnesses are shown in the middle. Optical characterization is performed by measuring the Mueller Matrix elements of the nanostructures to discriminate the chiral effect from the co-existing optical anisotropy [4]. As an example, we present in Figure 1 the chiral optical responses of two complementary structures.

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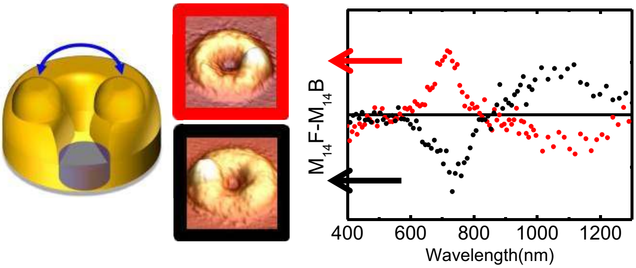

Figure 1: Left: sketches of the proposed 3D nanostructures. The position of the top dot can be controlled in order to tune the chirality of the structure (blue arrows). Middle: representative AFM images of two structures with complementary handnesses. Right: complementary spectra representing the chiral optical responses obtained from the Mueller Matrix elements.

In Vivo Protein Corona Formation on Gold Nanoparticles of Various Size and Shape

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Abstract

Protein corona formation is a well-known process that modifies the identity of nanoparticles upon contact with the biological milieu, thereby affecting their *in vivo* performance. Although most studies are carried out *in vitro*, these conditions do not accurately represent the *in vivo* situation. Our study is thus focused on protein corona formation around gold nanoparticles (AuNPs) *in vivo*. The aim of this research is to achieve a better understanding of how protein corona is influenced by the size and shape of NPs. For this purpose, gold nanorods (AuNRs) and gold nanostars (AuNSts) of 40 and 70 nm of size were intravenously injected in CD-1 mice, recovered by cardiac puncture and then separated from unbound plasma proteins. Physico-chemical characterization of nanoparticles before and after protein corona formation was performed by Dynamic Light Scattering (DLS), UV-Visible Spectroscopy and Transmission Electron Microscopy (TEM). Protein coronas were quantitatively and qualitatively characterized by LC-MS/MS. Our results show that both, size and shape, have an impact on both the amount of adsorbed protein and the composition of the protein corona in the case of *in vivo* corona. This study is expected to open a full method of analysis that is closer to real world applications of nanomedicine.

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Carbon NanoDots: New NanoCarriers for Drug Delivery

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Tremendous progress over the past decades in the field of nanomedice emerged constantly. However, the development of water soluble drug delivery systems is still an urgent need, and resource intensive endeavor that is not always guaranteed to result efficacious drugs. Herein, we report a new avenue to change the landscape of future drug carriers based on Carbon NanoDots (CNDs), a fascinating class of recently discovered nanocarbons that comprises quasispherical nanoparticles with sizes below 10 nm. They typically display excitation wavelength dependence, good biocompatibility, high water solubility, and low toxicity, among others.[1] Due to these excellent properties, CNDs have gained tremendous attention in nano-mediated cancer delivery and targeting.[2] In this work, a simple bottom-up approach to obtain CNDs from carbon and nitrogen sources and employing a microwave reactor is described.[3] The resulting CNDs were functionalized with a low water soluble drug, Taxol® (PTX). Moreover, we have studied the potential of the CNDs-PTX nanocarrier against different cell lines.

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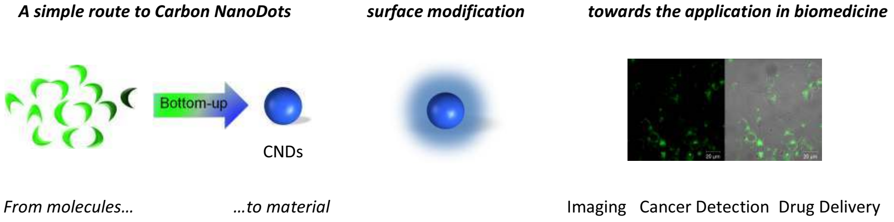

Figure 1: Schematic representation of the synthesis of CNDs and their bioapplications.

Femtosecond Laser-Controlled Tip-to-Tip Assembly and Welding of Gold Nanorods

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The unique collective optical properties that arise when plasmonic gold nanocrystals are in close proximity depend strongly on the rational design of the self-assembly procces.[1,2,3] In this context, one of the most efficient methologies to achieve nanoparticles assembly relies on the use of dithiolated molecular linkers.[3] In direct analogy to molecular polymerization, the chain growth process through the formation of initial short oligomers which then elongate producing a broad population of aggregates. However, this mechanism renders highly polydisperse samples which make are hard to use for applications in nanoplasmonics. Based on the irradiation with low fluence near-infrared (NIR) femtosecond laser pulses, we propose a novel route to obtain selected plasmonic oligomers in high yields.[4] Herein, we synthesize gold nanorods of which octanedithiol mediated tip-to-tip assembly leads to formation of trimers in optical resonance with a 800 nm Ti:sapphire femtosecond laser. Thereupon, irradiation with fs pulses induces the formation of hot spots that favor the photothermal decomposition of the interparticle molecular linkers. Consequently, rupture of the trimers takes places meanwhile dimers, which are not in resonance with the laser, remain intact. Furthermore, when the laser energy exceeds certain threshold, melting and welding of gold nanorod through the tips occur, offering a new pathway to forge plasmonic species with optical response at the NIR.

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Atomistic modeling of adsorbed thiolates on Au nanoparticles (GNP). Study of the effect of the capping layer on the GNP's melting temperature.

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Metallic nanoparticles are perhaps one of the most outstanding applications of nanotechnology due to the imminent use of these nanostructures on diverse fields, i.e. biosensors, catalysis, drug "delivery" and construction of nano-circuits [1].

Preparation, conservation and protection of metallic or multimetallic nanoparticles require protection with organic ligand molecules if they will remains in a colloidal suspension. When nanoparticles are made of gold, a relatively easy way of protect them is through organic molecular self-assembly, particularly with thiolate molecules due to the strong interaction between sulfur and gold atoms. Self-assembly monolayer's (SAM's) have been intensively studied, at experimental and theoretical level, on extended gold (111) surfaces and small Au clusters. Nevertheless, a clear understanding about some fundamental structural aspects of passivated Au nanoparticles in the range of 1-30 nm still does not exist.

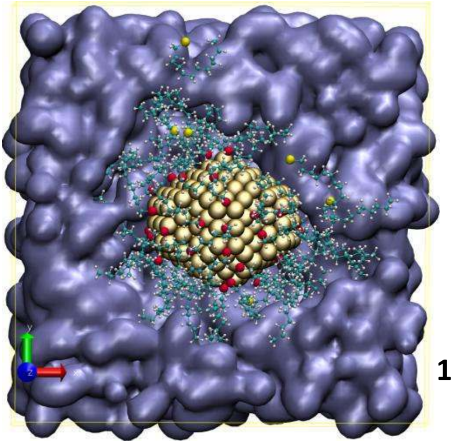

Figura 1: GNP (309 Au atoms) in gold-yellow. Thiolate molecules: S [Yellow (adsorbed), Red (Desorved)]. Alkyl chain in cyan (C) and white (H). Hexane solvent in continuos iceblue.

In the present work we evaluate the effect on melting temperature on GNPs where the defects induced by thiolate capping on the metallic surface are not negligible. With that in mind we have developed a many-body potential compatible with TB-SMA, to take into to account the most archetypical adsorption sites of thiolates on gold [2]. Molecular Dynamics simulations are performed to compute the thermal behavior of GNP covered with alkane thiolate on hexane. The melting point if correlated as a function of the length of thiolate alkyl chain and compared to the particle only in solvent and in vacuum [3]. The new semiempirical framework which is implemented in the TINKER code.

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Sensitivity Limit of Nanoparticle Biosensors in the Discrimination of Single Nucleotide Polymorphism

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Single-nucleotide polymorphism (SNP) is a random replacement of a nucleotide in a given genetic location that occurs in human genome at every few hundred of bases across the genome[1]. These replacements alter functioning of proteins, leading to cancer, cardiovascular or neurodegenerative diseases[2]. Therefore, the ability of sensitive detection of specific SNPs has considerable value in diagnosis, prediction of patient's responses to treatments, and risk of relapse of diseases. LSPR-based detection methods offer some significant advantages: applicability to a wide range of analytes, ease of use, elimination of the use of toxic organic solvents, point-of-care applications, as well as high sensitivity in the detection of some biological species[3].

The main factor limiting colloidal sensor sensitivity is the number of available target DNA molecules able to aggregate nanoparticles and therefore produce an optical output. A systematic study for SNP detection using AuNPs of 13, 46 and 63 nm using conventional sandwich assay is proposed[4]. It has been found that by increasing particles diameter at constant gold concentration, one can improve limit of detection by two orders of magnitudes (Figure 1). At constant gold concentration and varying particles size, the best sensitivity was reached with the large particles, 63 nm. This tendency was explained by a higher ratio of target-to-particles as compared to the smaller AuNPs. Using 63 nm particles we could differentiate match from mismatch sequences down to 10 pM. The results show that colloidal biosensors based on the aggregation possess an intrinsic limitation which is the number of target molecules per particles.

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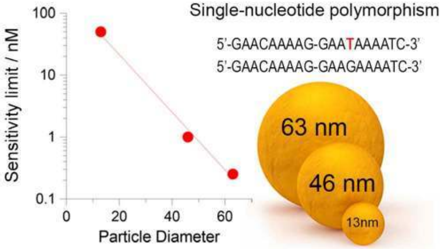

Figure 1: Sensitivity limit versus particle size, showing a linear dependence in a logarithmic scale.

Development of nanostructured host-guest hybrid material for Non-Linear Optics

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One approach to achieve photoactive hybrid materials with interesting properties for optical applications consists on the encapsulation of organic fluorophores into rigid inorganic frameworks. In this sense, it has been demonstrated that MgAPO-11, a magnesium aluminophosphate with AEL structure and 1-D nanochannels, is a suitable host to guest dyes with a general molecular structure built up by three fused aromatic rings since it prevents dye aggregation due to its the tight pores (6.5 Å x 4 Å) with special topology, consisting on pockets.[1,2] Also due to the narrow size of the channels, the incorporation of the dyes should be carried out by crystallization inclusion method instead of by the typical post-synthetic approaches since diffusional process is impeded.

In order to find new nanostructured materials with applicability in the field of non-linear optics, a dye with intrinsic non-linear optical properties was chosen to be occluded into the MgAPO-11 matrix, the LDS 722. Although the synthesis of this type of dye-loaded MgAPOs is rather straightforward, an optimization of the synthetic procedure was required for the incorporation of this dye. Finally, the result was pure LDS722/AEL material which shows enhanced fluorescence capacity in comparison with the dye in solution (ϕ_{fl} (dye in aqueous solution) ~ 0.01 *vs.* ϕ_{fl} (LDS722/AEL) = 0.55) and highly anisotropic response to the linearly polarized light due to the preferential alignment of the dyes within the tight pores. As a result, this material revealed attractive second-order non-linear properties such as Second Harmonic Generation (SHG) under NIR irradiation, proven through microscopic techniques at single crystal level. [3]

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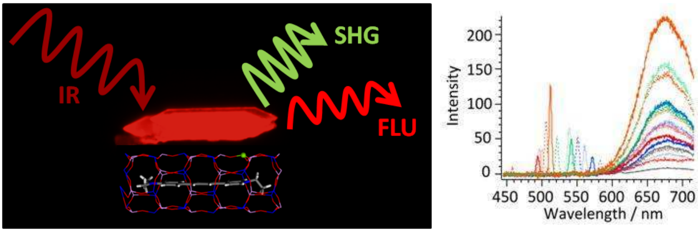

Figure 1: Left: Fluorescence image of a LDS722/AEL crystal with an illustration of the processes arising under NIR illumination. A representation of the LDS 722 molecule within an AEL channel is also shown (down). Right: SHG/Fluorescence spectra of a LDS722/AEL single particle upon different excitation wavelengths from 812 to 1222 nm.

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Design and Fabrication of Photonic Bands in Nanoporous Anodic Alumina-based Rugate Structures

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Rugate structures (RS) are one-dimensional photonic crystals with a continuous and periodic variation of its refractive index with depth. They can be obtained on the basis of nanoporous anodic alumina (NAA), formed by the electrochemical anodization of high-purity aluminum by means of a sinusoidal anodization current [1]. The sinusoidal modulation of the refractive index results in an interesting optical behavior consisting of a well-defined photonic stop band. Furthermore, several sinusoidal profiles can be overlapped in order to produce films with several forbidden phonic bands [2 ,3].

The optical properties of NAA-RS can be engineered by adjusting several design parameters such as the average anodization current, the current amplitude, the period and the number of periods of the sinusoidal current component. This way, high quality and selective photonic bands located in the ultraviolet (UV), visible and near infrared (NIR) range can be precisely defined.

In this work, we design and fabricate NAA-RS with photonic bands in the UV and VIS, a spectral range especially interesting for photonic applications like sensing and data coding. We make a systematic study of the influence of each design parameter on the optical properties of NAA-RS, emphasizing the influence of the design parameters on the quality factor and position of the photonic stop band. An example is shown in Figure 1a, where the influence of one of the design parameters (period length) on the position and width of the photonic bands of NAA-RS is observed.

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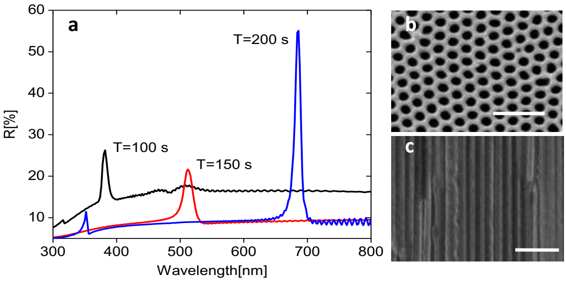

Figure 1: (a) Reflection spectra of NAA-RS with different sinusoidal period (T), and SEM images of a NAA structure: (b) top view and (c) transversal view. Scale bar: 500 nm.

Functionalized Gold-based Nanostructures for Uveal Melanoma Treatment [1]

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Uveal melanoma is a rare disease accounting for 5% of all melanomas and 0.1% of all cancer deaths. It is the most common primary intraocular malignant tumor in adults resulting in liver metastasis in 85% of the cases, half of which end up in death. This overwhelming scene has raised up a considerable interest in the development of novel approaches for the treatment of such disease.

One of the biggest problems regarding cancer therapeutics is the lack of specificity of the chemotherapeutic approaches. Functionalized gold-based nanostructures may offer a strategy to overcome such complications taking into account the low toxicity and the high cellular penetration capacity of gold nanoparticles, which make them an excellent choice for biomedical applications [2].

We have tested functionalized gold nanoparticles (AuNPs, Figure 1.A) and albumin-stabilized gold nanoclusters (BSA-AuNCs, Figure 1.B) as delivery systems for two chemotherapeutic agents (AZD8055 and Selumetinib, Figure 1.C) in several uveal melanoma cell lines. These two drugs interfere with the MAPK and the PI3K pathways, respectively, which are involved in the development of uveal melanoma promoting cellular growth, proliferation, invasion and cell survival.

Our results show that Selumetinib and AZD8055 gold-based nanostructures are suitable for delivery systems in several uveal melanoma cell lines, reducing cellular viability in a similar way to the free drugs. Due to the versatility of these nanomaterials, we are assessing different approaches to improve their selectivity and efficacy as drug carriers.

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Figures

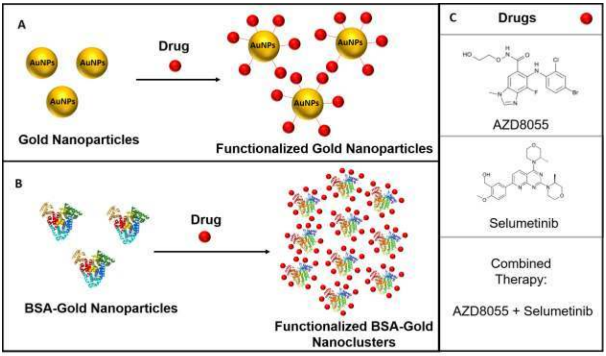

Figure 1: Functionalization of gold-based nanostructures for drug delivery. A. Drug functionalization of gold nanoparticles. **B.** Drug functionalization of BSA-Gold nanoclusters. **C.** Drugs tested for uveal melanoma treatment: AZD8055, Selumetinib and combined therapy.

Valorization of activated saline slags as adsorbents for the removal of acid dyes from aqueous solutions

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Abstract

This work describes the surface properties of activated saline slags generated during aluminium recycling processes and the application of these materials as adsorbents for the removal of Orange II and Acid Blue 80 from aqueous solutions. Saline slags were chemically treated with 2 mol/dm^3 aqueous solutions of HCl, H_2SO_4 and NaOH for 2 h using a reflux system. The solids were characterized by nitrogen adsorption at −196°C, X-ray diffraction and ammonia pulse chemisorption at 70°C. The chemical treatment reduces the textural properties of the saline slag (see Figure 1-A) and increases the adsorption capacity of ammonia in the case of acid activated solids. Considering the adsorption capacity of these materials, it is observed that the saline slag treated with HCl adsorb rapidly and all the amount of dyes present in solution. The other materials can retain between 50 and 70% of the molecules present in solution. The kinetic (see Figure 1-B) and equilibrium results have been fitted using several mathematical models. The results showed that activated saline slags can be used as adsorbents in wastewater treatment for the removal of organic contaminants.

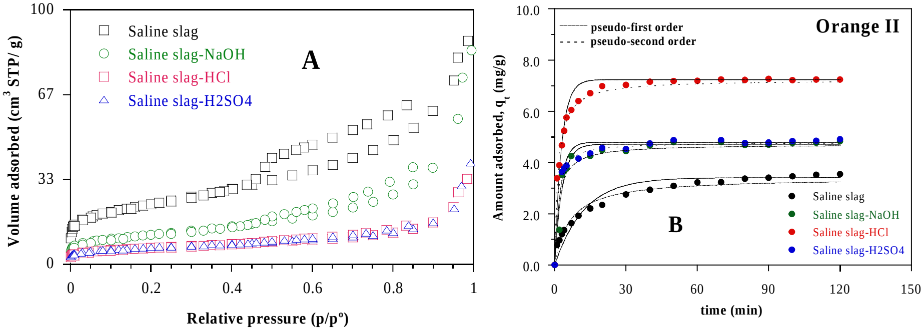

Figure 1: **A**-Nitrogen adsorption at −196°C. **B**-Experimental (symbols) and model (lines) for the kinetic adsorption of Orange II on the activated saline slags.

Acknowledgements

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Molecular impact of functionalized nanodiamonds on *ex vivo* human immune cells response

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Abstract

Carbon-based nanomaterials have been explored for biomedical applications due to their unique physicochemical properties [1]. In this context, nanodiamonds (NDs) are gaining increasing interest thanks to their biocompatibility, structure and unique electrostatic properties for several nanomedicine applications such as drug delivery, bioimaging and cancer therapy [2,3,4]. However, before any effective application of NDs, their action on the immune system is not fully clarified yet [5]. Nowadays, no comprehensive studies were performed on the immune system with NDs. In this work, we propose an integrative characterization of the molecular impact of two different types of NDs, Oxidized (-Ox) and Aminized (-NH_2), on several human immune cell subpopulations such as T and B Lymphocytes, Natural killer (NK), monocytes and on red blood cells (RBCs). Both NDs showed no toxicity on RBCs and on the T and NK lymphocyte subpopulations. Only monocytes and B cells were affected by the presence of NDs-Ox at the highest concentration used while the functionalized ND-NH_2 counterpart showed no toxicity also on these cell types. NDs-Ox exposure increased proinflammatory cytokines secretion, such as IL6, IL1β, TNFα and IL10, while we found a reduced immune cell activation in -NH_2 treated samples. On monocytes, -NH_2 showed low levels of CD25 activation marker expression compared to -Ox. To deeply analyze the molecular immune impact of NDs a gene expression analysis of 84 immune genes was performed. Intriguingly, after 24h -NH_2 reduced the expression of genes related to a strong inflammatory response such as IL10, IL5, IL4 compared to the -Ox form. These results emphasize the importance of the amino group functionalization, enhancing the biocompatibility of ND-based nanomaterials. These data are of particular interest for further translational applications of amino-functionalized NDs being possible inert materials useful for drug delivery and bioimaging applications.

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INSPIRED – A project to print the future

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The INSPIRED project, acronym for "INdustrial Scale Production of Innovative nanomateRials for printEd Devices", is funded under the EU Framework programme for Research and Innovation HORIZON 2020.
The focus of INSPIRED is to fundamentally improve the current understanding of Printed Electronics (PE). PE is set to revolutionize the electronics industry over the next decade and can offer Europe the opportunity to regain lost market share. It allows for the direct printing of a range of functional ink formulations to enable a simpler, more cost-effective, high performance and high volume printing processing in comparison to traditional circuit board and semiconductor manufacturing techniques. The move towards low-cost, liquid-based, high throughput techniques, such as inkjet printing, requires that suitable functional inks are available for end users. Presently there are issues with the supply of industrially relevant quantities of nanomaterials which are low cost, high performance, environmentally friendly and tailored for high throughput systems. INSPIRED will address these challenges.

By covering the whole value chain from nanomaterial synthesis and scale-up over printing process R&D and equipment manufacture to applications development, the INSPIRED partners will ensure the availability of nano-based functionalised inks in industrial scale quantities and enable rapid and high-throughput production of novel printed electronic components on a wide variety of substrates.

In detail, the INSPIRED project will develop the following Pilot lines

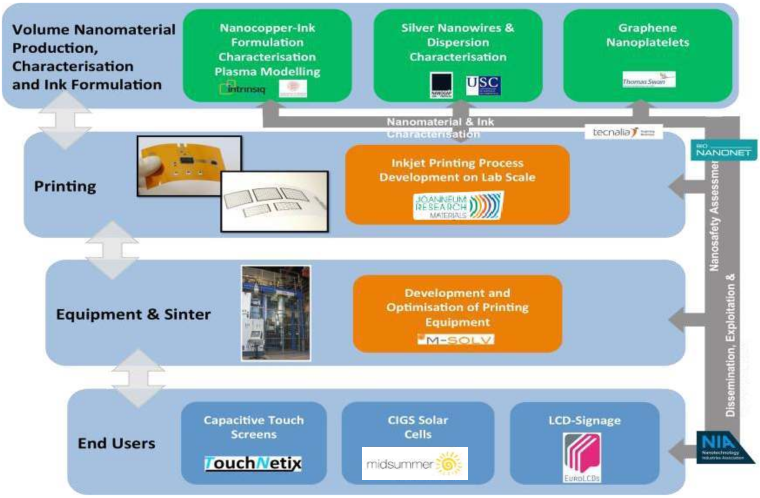
- ***Materials, their formulations and scale-up:***
  - From synthesis to formulation
    - Nano-copper
    - Ag Nanowires
    - Graphene materials
- ***Processes:***
  - High-volume printing and sintering including development of pilot equipment
  - Development of simplified manufacturing process (One step Interconnect, OSI) as an alternative PV interconnect method
- ***Devices (exemplar applications):***
  - Capacitive touchscreens using copper inks / AgNWs
  - LCD system using conductive inks - LC Display demonstrator
  - CIGS cells using copper inks / AgNWs/GNPs

The partners in the project, which has a duration of four years, come from academia, industries and organisations in 7 European countries and are experts in their fields, covering nanomaterial synthesis and scale-up, ink formulation, high throughput printing, equipment manufacture and process engineering, nanosafety assessment, process and post-process characterisation of nanomaterial inks and components as well as touchscreen display, LCD and CIGS PV cell design and manufacture. The project coordinator is Joanneum Research Forschungsgesellschaft mbH (Austria), who is supported by Intrinsiq Materials Ltd (UK). Further partners are NanoGap Sub-nm-Powder S.A. (Spain), M-Solv Ltd (UK), Thomas Swan & Co Ltd (UK), BioNanoNet Forschungsgesellschaft mbH (Austria), Touchnetix Ltd (UK), Midsummer (Sweden), EuroLCDs (Latvia), Nanotechnology Industries Association (Belgium), Alma Mater Studiorum-Università di

Bologna (Italy), Fundacion Tecnalia Research & Innovation (Spain) and University of Santiago de Compostela (Spain).
Tecnalia´s role in the project is devoted to the re-formulation and characterization of graphene inks, as well as settling the optimization of different processes like nanoAg coatings, screen-printing, ink-jet printing and sintering of Cu pastes and inks.

Further information on the INSPIRED project can be found at the project website: www.nanoinspired

Figures



Novel functionalization reactions of Graphene on surfaces

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Since the production and characterization of graphene mono- and few-layers, much effort has been directed toward the chemical functionalization as a tool for tuning graphene chemical and physical properties.[1] Besides, a controllable graphene modification is a mandatory step for the grafting of functional biomolecules, like DNA or proteins, which are often used in bioelectronics.[2]

This work is focused on the development of chemical modifications on the graphene surfaces based on covalent approaches in order to produce stable components for biomedical devices. In particular, we have addressed low aggressive novel functionalisation strategies based on cycloaddition and radical reactions. In addition, we have also explored the influence of different substrates on the reactivity behaviour of graphene.

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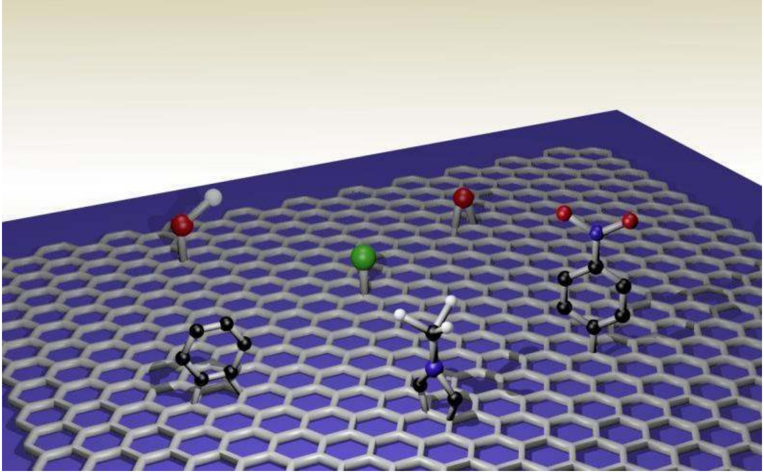

Figure 1

Growth and characterization of chiral gold nanorods

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Nanostructures with plasmonic functionalities have become an active topic of research. By controlling morphological parameters, optical properties of the nanostructures can be tailored with the applications in, for example, biosensing and gas areas and in integrated photonic devices for telecommunications.

Considering the fabrication, hole-mask colloidal lithography (HCL) is a versatile method to produce randomly distributed nanostructures in large areas (over cm^2) such as discs, rings and crescent-shaped structures [1], as well as magneto-optically active nanostructures by combining noble metals with ferromagnetic metals.

In this work we present a complex structure formed by two gold nanorods [2] separated by a dielectric calcium fluoride (CaF_2) layer in a chiral configuration obtained by HCL.

Morphological properties of the nanostructure are studied with Atomic Force Microscope (AFM) and the optical properties are analized using the Mueller matrix elements in transmission, which allow discrimitation between optical anisotropy and chiral effects.

Eventually, ferromagnetic components will be added into the system, and the response of the structure in the presence of magnetic field will be presented.

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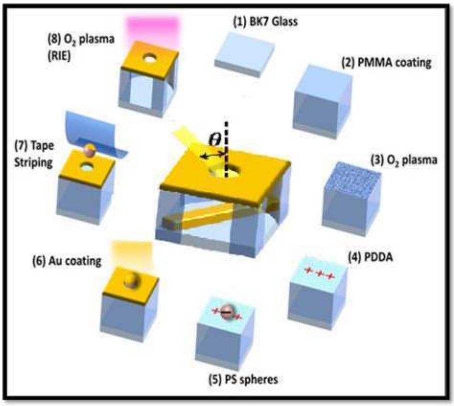

Figure 1: Diagram illustrating the basic process steps and resulting structures produced with HCL nanofabrication.

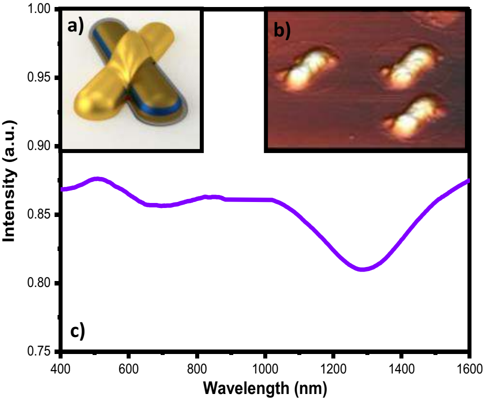

Figure 2: a) Schematic representation of some of the structures: Au rod on top of a Au/Co/Au nanorod. **b)** AFM image of crossed gold nanorods placed at 45 degrees each other **c)** Transmission spectrum of the sample shown in figure 2b.The dips are related with the plasmon resonances of the structure.

Intense UV and visible up-conversion luminescence from SiO_2-$BaGdF_5$ glass-ceramics doped with Yb^{3+}/Er^{3+}, Yb^{3+}/Tm^{3+}or Yb^{3+}/Er^{3+}/Tm^{3+}

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UV-visible up-conversion luminescence of materials doped with rare-earths (RE^{3+}) ions has attracted great interest due to their applications in areas such as temperature sensors, solid state lighting, solar cells, biomedical image and so on [1,2]. Herein we study the up-conversion properties of $BaGdF_5$ nanocrystals doped with Yb^{3+}/Er^{3+} and Yb^{3+}/Tm^{3+} pairs of ions. The sol-gel method, allowed us to obtain the precursor glasses that by adequate thermal treatments given rise to the glass-ceramics containing single-phase and homogeneous RE^{3+}-doped $BaGdF_5$ nanocrystals. X-ray diffraction measurements confirmed the precipitation of cubic phase $BaGdF_5$ nanocrystal with cell parameter that varies as function of dopant concentration. Up-conversion luminescence reveals an efficient absorption around 980 nm, leading to intense UV and visible emissions, confirming an energy transfer up-conversion (ETU) mechanism responsible for the observed luminescence as well as the "saturation effect". Additionally, color tuneability was quantified, in Yb-Er-Tm triply doped glass-ceramics, in terms of CIE diagram, and in particular a white colour, close to the standard equal energy white light illumination point, has been achieved for a certain thermal treatment.

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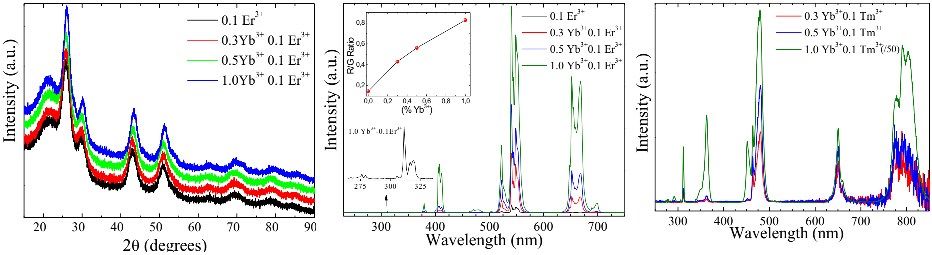

Figure: (a) XRD patterns of xYb^{3+}-Er^{3+}-doped SiO_2-$BaGdF_5$ nGCs, where x=0, 0.3, 0.5 and 1.0, heat-treated at 650 ºC. (b) Up-conversion emission spectra in xYb^{3+}-Er^{3+}-doped SiO_2-$BaGdF_5$ nGCs (mol %) heat-treated at 650 ºC, under 980 nm excitation at 300 mW pump power. (c) Up-conversion emission spectra in xYb^{3+}-Tm^{3+}-doped SiO_2-$BaGdF_5$ nGCs (mol %) heat-treated at 650 ºC, under 980 nm excitation at 300 mW pump power.

Characterization of the toxicity of high-generation cationic PAMAM dendrimers towards a representative organism of aquatic ecosystems

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Nowadays, nanomaterials are widely used in many different fields as biomedicine. Dendrimers are nano-sized, radially symmetric molecules with well-defined, homogeneous, and monodisperse structure that has a typically symmetric core, an inner shell, and an outer shell; due to these characteristics, their use is being tested in the implementation of targeted therapies in biomedicine. Today, hundreds of products containing nanomaterials are used around the world which could end up in aquatic ecosystems [1].

This work has focused on analyzing the effect of poly (amidoamine) (PAMAM) G5-NH_2 and G7-NH_2 in an organism of great ecological importance such as the filamentous cyanobacterium *Anabaena* sp. PCC7120.

Nanoparticles have particular characteristics that depend on various physicalchemical properties such as size and aggregation. Firstly, physicochemical properties of both dendrimers were measured in water and culture medium. Both dendrimers in culture medium showed an elevated level of aggregation (measured with DLS) and displayed a positive charge (measured as z-potential).

Then, the effect of both dendrimers was studied. Both dendrimers significantly decreased the growth of the cyanobacterium. G7-NH_2 (EC_{50} = 0.072 ± 0.005 µM) was more toxic than G5-NH_2 (EC_{50} = 0.096 ± 0.004 µM). There was a clear relationship between dendrimer generation and toxicity, with higher toxicity for higher generation, as previously reported [2].

Physiological parameters were studied by flow cytometry using several fluorochromes to elucidate toxicity mechanisms. Cyanobacteria exposure to dendrimers resulted in significant increase in the formation of intracellular reactive oxygen species (superoxide anion, hydrogen peroxide and hydroxile anion), increase of lipid peroxidation, damage in membrane integrity, membrane potential depolarization, increase of metabolic activity, acidification of intracellular pH and alteration of intracellular free Ca^{2+} homeostasis.

Morphology of the cyanobacterium was studied by optical microscopy and flow cytometry. The results showed alteration in the morphology of both filaments and individual cells within filaments exposed to dendrimers.

Photosynthesis was analysed in the cyanobacterium exposed to dedrimers. Both dendrimers significantly increased photosynthetic O_2 evolution, as previously described in other organisms [3]. Furthermore, the in vivo analysis of pigments showed an increase in the fluorescence of chlorophyll a, phycocianin and carotenoids. Finally, the expression of genes related to oxidative stress response were analysed. Genes encoding superoxide dismutase (*sodA*) and peroxidases (*prxA* and *prxQ-B*) increased expression after exposure to both dendrimers.

Dendrims exhibited high toxicity towards *Anabaena* sp. PCC7120 and several physiological, morphological, photosyntethic and genetic paramenters were affected, so this study provides relevant data to advance in the field of nanomaterials environmental risk assessment.

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Plasmonic effects observed in Transparent Conductive Oxides (TCOS) thin films

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Plasmon resonance, owing to the collective oscillation electrons in response to an applied electromagnetic field, is a phenomenon observed in metals and semiconductors. In semiconductor the plasmonic energy and plasmonic frequency can be tuned from the far infrared towards the visible range [1]. Nowadays this property is a developing field with application in plasmonic based devices such as waveguides, solar cells and smart windows [2].

Heavily doped transparent conductive oxides (TCOs) are degenerated semiconductor that are being investigate, both in thin film and colloidal forms for plasmonic applications [3]. Several TCOs based on indium, tin and zinc oxides have been prepared by magnetron sputtering at room temperature on glass substrates, changing different deposition parameters (discharge power, oxygen content or deposition time), and subsequently annealed in different atmosphere. They have been analyzed by X-ray diffraction, spectrophotometry, and Hall measurements; taking into account that the structural and electro-optical characteristics of such metal oxide coatings are highly related and depend on the deposition parameters apart from the material composition [4]: In this work, the plasmonic effect as a function of the annealing temperature in N_2 N_2/H_2 and air atmospheres of TCOs films have been analyzed comparatively. The purpose has been to achieve transparency in the visible range combined with high electrical conductivity, and an associated plasmon absorption in the near-infrared region. Besides the plasmonic characteristics (plasmon resonance position and width) determined by spectrophotometry have been related to the charge transport parameters (carrier concentration and mobility) obtained also by Hall-effect measurements of the same samples. The final objective is to get a better knowledge of the relationship between the microstructure and the electrical-properties, which can contribute to a further development of these transparent conductive oxides.

This work has been supported by the project MAT2015-66649-R (MINECO/FEDER).

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Figures

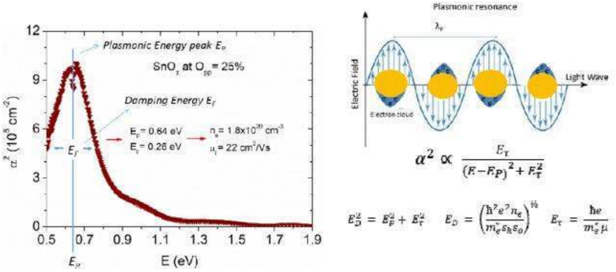

Figure 1: Plasmonic resonance effect in as-grown SnO_{2-x} thin film prepared by DC-magnetron sputtering

Unraveling the nature of NIR resonant nanoparticles

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Since the first report on plasmonic nanoparticle-based photothermal tumor therapy, several nanoparticle structures have been developed with one main focus: to tune the plasmon resonance frequency into the near-infrared window of biological tissue. One method proposed to create such nanoparticles relies on the reduction of gold salt by sodium sulfide. The formation of a strong NIR extinction peak was observed, the origin of which has been matter of a longstanding debate. By means of HRTEM and X Ray absorption techniques we have characterized the products of this controversial synthesis. Only metallic gold nanostructures are formed, mainly icosahedrons and very thin triangles. Different reduced sulfur species are adsorbed on the particles, mostly sulfides and polysulfides, similarly to what is found on planar gold surfaces. Therefore this precludes the idea that oxidized sulfur species are the actual reducing agents for Au(III) ions.

To shed light on the type of nanoparticle responsible for the NIR resonance we developed a new sorting method capable of distinguishing different nanostructures by using their strong scattering force to print them at specific locations onto hard substrates. By arresting the synthesis at different times, and using focused lasers whose wavelengths were tuned to the respective resonances, we are able to separate the nanoparticles based on their plasmon resonances. This enables us to acquire single particle Rayleigh scattering spectra and compare those with the morphology of the nanoparticles obtained through scanning electron microscopy. We found that the thin gold nanotriangles are responsible for the observed NIR resonance.

Knowing the size and shape of the NIR resonant particles and the species adsorbed to their surfaces enables us to develop accurate strategies for purification and post functionalization to anchor biomolecules that can improve the efficiency and applicability of cancer treatments.

Figures

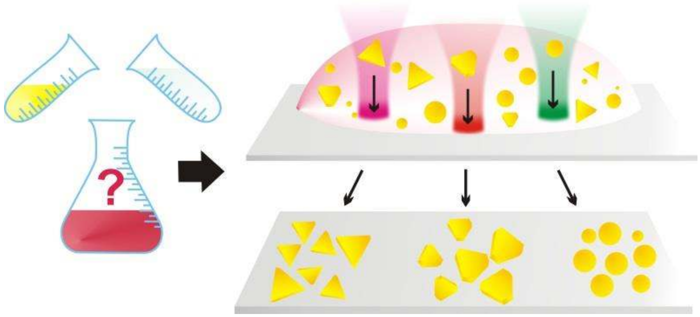

Figure 1: Scheme of the synthesis of gold nanostructures and the optical sorting method by their plasmon resonance.

Radio-frequency figures of merit of graphene transistors supported on hexagonal boron nitride substrates

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Hexagonal boron nitride (hBN) has been demonstrated to be an appropriate substrate for graphene devices, which has led to a huge increase in graphene device quality [1]. Given that, it seems timely to investigate if this increment in quality could be exploited in transistors to get competitive RF performances. So, in this work we have explored the scalability of these devices. For such a purpose, we have applied multi-scale physics based techniques to estimate the RF figures of merit. The information on the carrier density dependent mobility and saturation velocity comes from an ensemble Monte Carlo simulator which deals with the relevant scattering mechanisms [2,3]. That information is fed into a self-consistent simulator, which solves the drift-diffusion equation coupled with 2D Poisson's equation [4]. That way we get the DC characteristics, which have been benchmarked against experimental data from our own GFET devices. From DC information we have calculated the parameters entering in a small-signal model valid for high-frequencies, which finally allows getting an estimate of RF figures of merit. Moreover, we have applied microwave engineering techniques to assess the stability of GFETs when the transistor is operated as an amplifier. We have found that, in order to reach the THz regime, scaling the device and maximizing the mobility of carriers in graphene could be insufficient, since the transistor functioning as a power amplifier may be unstable. So care must be exercised when the device is designed, and we have found that the choice of the bias point is critical. We have also quantified the impact of gate series resistance and the role played to improve RF performance, especially in the short-channel case.

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NanoPilot project: A Pilot plant for the production of Polymer based Nanopharmaceuticals in Compliance with GMP

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Nanomedicine is expected to gain in importance in the near future, especially in the field of drug-delivery, where the use of nanovehicles could: a) increase the availability of an active pharmaceutical ingredeints (API); b) target specific sites of action with a direct benefit in the reduction of side effects and increase of efficacy; c) deliver drugs across biological barriers; d) combine several drugs with synergic effects in the same vehicle, and; e) combine imaging and therapy in the same carrier[1]. There are some marketed nanotherapeutic products for parenteral and oral administration [2] and more under development. In addition, other administration routes will be probably accessible in the near future according to preclinical and clinical investigations, as for example, ocular, pulmonary, nasal, dermal or vaginal [3]. It is time to push those promising developments to the clinical stage, i) generating robust and translatable manufacturing processes, ii) completing full toxicological preclinical studies and iii) validating those new nanopharmaceuticals in clinical trials. This statement will be only possible if technology developers can easily validate their manufacturing processes and scale them up according to regulation requirements.

NanoPilot, is a H2020 funded EU project that will cover this need by setting-up a pilot plant operating under Good Manufacturing Practice (GMP) for the production of small batches of polymer-based nanopharmaceuticals under GMP. The pilot plant has been designed to be flexible and work in campaign to produce a wide range of nanopharmaceuticals. Quality System has been already implemented and Nanopilot Pilot Plant will apply for the first GMP manufacturing authorization in 2017 for non-sterile lyophilisates. At the end of the project sterile lyophilisates and liquids would be also produced. Three different nanopharmaceuticals production processes are being implemented in the frame of the project to apply for those authorizations:

a) A short interfering RNA (siRNA) for the treatment of ocular pain associated with dry eye syndrome.
b) HIV nanovaccine that combines different peptides in its formulation.
c) Hyaluronan based particles, for the treatment of interstitial cystitis/painful bladder syndrome (IC/PBS).

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Figures

Figure 1: Nanopilot: A project to move forward Nanomedicine from Lab to Clinical trials

Advanced nano-electric characterization with atomic force microcopy characterization of 2-d materials and nano-devices

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Over the past 30 years, Atomic Force Microscopy has evolved from a microscope to measure just the surface topography to a wide variety of measurement modes that provides a way to characterize other atomic interactions or physical properties like magnetic field, electric field, nanoscale dissipation processes, thermal conductivity, electrical conductivity, resistance, surface potential, piezoresponse, Young modulus,… Electrical nanocharacterization with AFM has emerged as a powerful tool to map electrical properties at the nanoscale, like surface potential (work function), local conductivity, . However, traditional setups in AFM make difficult to obtain accurate and repeteable results over several types of samples.

In this poster we will show the capabilities of the last developed AFM modes for electric nanocharacterization: High Definition Kelvin Force Microscopy (HD-KFM), ResiScope, Soft Resiscope (local resistance in intermittent contact), and Scanning Microwave Impedance icroscopy (SMIM) and Raman Spectroscopy. These new modes overcome the intrinsic difficulties of electrical nanocharacterization with AFM both in smooth surfaces like 2-D materials (graphene, MoS2, metallic nanoparticles, and over increased challenging samples like perovskites solar cells, transistors or nano-devices.

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Figures

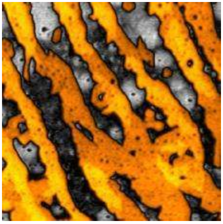

Figure 1: Surface Potential image of graphene(orange 1 ML, yellow 2ML) on silicon carbide (grey)

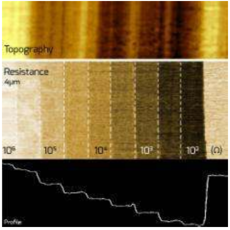

Figure 2: Topography and resistance images of substrate with different dopant levels of ionic implantation.

Transcriptional changes induced by in vivo exposure to multi-walled carbon nanotubes (CNTs) in Chironomus riparius (Diptera) aquatic larvae

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The widespread use of carbon nanotubes (CNTs) in the industry and biomedicine provokes their dispersion in the aquatic environment through sources such as disposal of CNT-containing consumer products, waste discharges and accidental spills. CNTs are hydrophobic and nonbiodegradable in the nature, these materials can accumulate in sediments into aquatic environments. At present, the studies of the effects of CNTs on aquatic organisms are scarce. The main objectives of the present study were to investigate the toxicity of multi-walled carbon nanotubes (MWCNTs) and to evaluate the effects of carbon nanotubes at genomic level using Chironomus riparius, a reference organism in aquatic toxicology. We analyzed the impact of CNTs on the activity of several genes related with DNA repairing mechanisms, cell stress response, cytoskeleton, and cell apoptosis. The transcriptional activity of the ataxia-telangiectasia mutated (ATM), X-ray repair cross-complementing protein 1 (XRCC1), heat shock protein 27 (hsp27), heat shock protein 70 (hsp70), actin and caspase 3 genes were evaluated by real time RT-PCR in C. riparius larvae after 24 hours of exposure to MWCNTs. The obtained results in the present work show the activation of caspase delay gene and the downregulation of hsp27, hsp70, and ATM genes at the highest tested concentration of MWCNTs. Moreover, the transcriptional activity of XRCC1 gene, related with excision-repair mechanisms, was not modified after MWCNTs exposure. These effects could be reflecting the activation of apoptosis by MWCNTs in C. riparius. Moreover, these data reinforce the need of further studies for the environmental risk assessment of this nanomaterial.

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Doxorubicin-loaded poly(ε-caprolactone) nanoparticles to improve drug antitumor effect

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Nanotechnology has provided new strategies in biomedicine for the treatment of certain pahologies such as cancer by the development of nanoformulations that transport antitumor drugs improving their solubility, specificity, half-life in blood stream and reducign their toxicity [1]. The tumor pathology more common diagnosed and the main cause of death worldwide for this desease is lung cancer [2]. One of the drug used to treat it is Doxorubicin (DOX) alone or in cobination with other drugs. This drug has a good antitumor activity. However, its low specificity for tumor tissues makes it toxic for non-tumor tissues causing severe side effects, especially cardiac toxicity [3].

Our study is based in the development of DOX-loaded poly (ε-caprolactone) (DOX-PCL) nanoparticles (NPs) that were tested in *in vitro* and *in vivo* lung cancer models. For the *in vitro* model we used human and mouse lung cancer cell lines A549 and LL/2. For the *in vivo* model immunocompetent C57BL/6 mice were subcutaneously inoculated with LL/2 cell line. Our results showed no toxicity of blank PCL NPs in general in any cell line thus demonstrating its biosafety and biocompatibility. Otherwise, DOX-PCL NPs increased cell death reducing the half-inhibitory concentration (IC50) compared to free drug up to 56.3% and 63.6% in A549 and LL/2 respectively (Fig. 1). Furthermore, *in vivo* assays demonstrated better antitumor activity (Fig. 2) and survival and also a reduction of cardiac toxicity in mice treated with DOX-PCL NPs. These results suggest that PCL NPs are a safe and efficient nanoformulation to improve the treatment of lung cancer.

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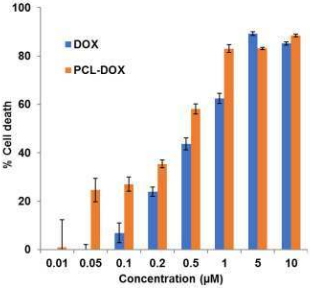

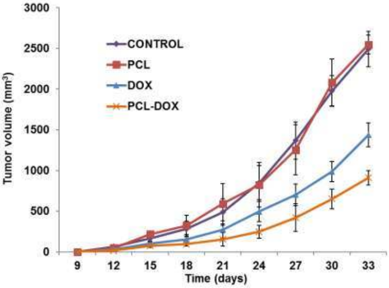

Figure 1: Percentage of A549 cell death.

Figure 2: Evolution along time of tumor volume of mice.

Graphene based Composites for Electronic Devices

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The aim of this work is to develop carbon fiber composites with higher thermal conductivity than conventional CFRP based on the use of thermally conductive carbon fibers as reinforcement and CNT and graphene as carbon nanofillers, as well as the use of high pressure as important processing parameter to compact the laminates.

The materials used to develop the high thermally conductive CFRP were (PF(S)-YS90A-140 carbon fabric of high axial thermal conductivity (300W/mK), (Weigh/area 140gr/m^2) from Nippon Graphite Fiber Corp. and MTM44 from CYTEC epoxy resin as matrix. Graphene "AvanGRP conductivo" from Avanzare was the carbon filler selected to introduce in the composite.

The key aspect on the manufacturing of high thermally conductive carbon fiber composites was the introduction of the graphene in the carbon composite laminate in an effective way.[1][2]

Figure 1 shows the graphene platelets deposited onto the carbon fabric by aqueous dispersion of graphene. Due to its size, they cannot pass through the carbon fabric (fiber diameter 10 micron).

Figure 2 shows the homogeneous dispersion of graphene into the resin.

Through thickness thermal conductivity was determined by Laser Flash Method. The maxima thermal conductivity is achieved by doping of the resin with 11%wt of graphene. (Table 1)

Acknowledgements

This work was supported by the ESA through the project THERCOBOX –Thermally conductive RTM carbon fiber reinforced polymer (4000107481/12/NL/CP).

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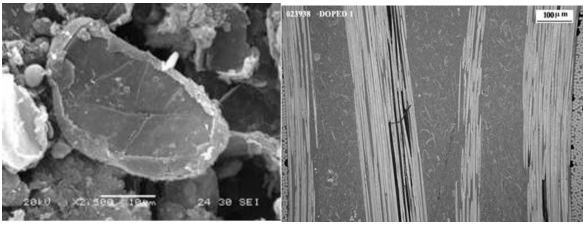

Figure 1: a)Graphene platelet onto carbon. b) CFRP laminates based on doped resin fabric.

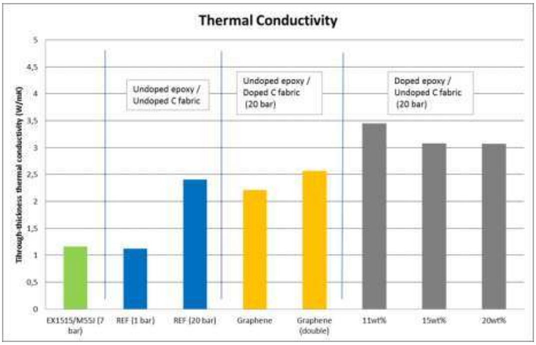

Table 1: Thermal conductivity of samples

Magnetization reversal in exchange coupled IrMn/FeCo patterned lines

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Exchange bias phenomenon arises from the interfacial coupling at antiferromagnetic/ferromagnetic (AFM/FM) interfaces and manifests as a unidirectional anisotropy on the FM, yielding a shift of the center of the hysteresis loop along the field axis known as exchange bias field (H_{EB}). The magnitude of the H_{EB} depends on the cooling procedure below the AFM Néel temperature. On the other hand, patterning of AFM/FM bilayers can modify the magnetic properties of materials inducing competing anisotropies. [1,2]

This work investigates the magnetization reversal of sputter-deposited polycrystalline IrMn/FeCo (AFM/FM) bilayers. In plane magnetization curves were measured at several angles by VSM magnetometry before and after an external field annealing for patterned and non-patterned bilayers. IrMn/FeCo lines were fabricated by physical etching of continous bilayers. The external magnetic field during annealing was applied parallel to the line axis.

The in plane angular dependence of hysteresis loops does not show any preferential anisotropy axis in as-grown samples, neither for non-patterned bilayers nor for patterned lines. The annealing of patterned and non-patterned samples originates exchange bias at room temperature. This procedure sets a clear unidirectional and uniaxial anisotropy along the external field direction, with a strong H_{EB} parallel to the line axis and null remanence and H_{EB} in the direction perpendicular to the lines. Magnetization reversal at different angular orientations is compared for patterned and unpatterned materials.

This work was supported by grants: EU FP7-IRSES-318901, Spanish MINECO FIS2013-45469 and FIS2016-76058, and CNEN, Fapemig, Capes, CNPq.

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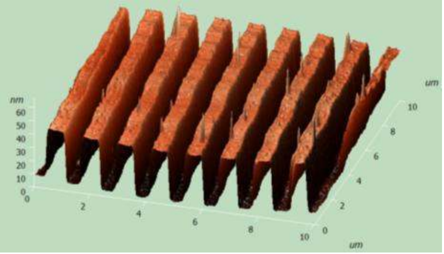

Figure 1: Atomic force microscopy image of patterned IrMn/FeCo bilayer.

Fabrication of lithographic nanoparticles for biomedicine

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The use of magnetic nanoparticles for biomedicine is a growing area of research and has shown promising results in several applications including drug delivery, hyperthermia and MRI. Magnetic behavior of nanomaterials strongly depends on their dimensions and geometry. In this sense Lithography techniques allow to design nanostructures with specific magnetic properties due to the possibility to tune the size and shape of magnetic materials in a controlled manner. Specifically, magnetic nanodiscs with spin vortex configuration are very promising for biological applications as they exhibit zero remanence so they do not agglomerate when they are dispersed in solution. Moreover, they rotate when an alternating magnetic field is applied. This mechanic oscillation was demonstrated to promote cancer cell destruction by the application of alternating magnetic fields of low amplitudes (100 Oe) and low frequencies (10's of hertzs)[1]. For this purpose vortex-state nanodiscs were fabricated by Interference Lithography, which allows to pattern large areas (cm^2) making possible mass production of nanoparticles. Our lithography system uses a Lloyd's mirror interferometer with a He-Cd laser (λ = 325nm) as a light source. Two fabrication routes were explored by using either positive or negative-tone resists that yield dot and antidot resist templates, respectively. These two fabrication strategies comprise several steps including thermal evaporation of Permalloy (NiFe) and the release of the nanostructures into solution. A full characterization of submicrometric discs (Figure 1) and a magnetic response analysis is discussed for each fabrication process comparing pros and cons for both strategies, which provide suitable lithographic nanoparticles for biomedical assays.

Work supported by grants: EU FP7-IRSES-318901, Spanish MINECO FIS2013-45469 and FIS2016-76058.

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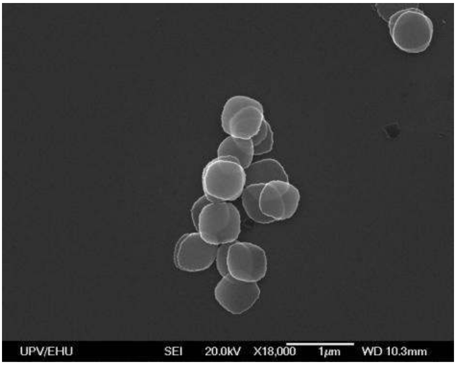

Figure 1: Scanning electron microscopy (SEM) image of released Permalloy disks dried on a Si substrate

Systematic study of Fe_3O_4 and γ-Fe_2O_3 nanoparticles for hyperthermia

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In order to improve the heating performance of magnetic nanoparticles during hyperthermia treatments, a systematic study of different Fe_3O_4 and γ-Fe_2O_3 nanoparticles has been done. There are a lot of parameters that take part in the processes of heating and the main purpose of this work is to compare different samples to investigate the relationship between heating efficiencies and physical properties such as coercive field, nanoparticle size and composition.

Nanoparticles with sizes between 6 and 300 nm with different coatings and synthesis routes have been analized. Magnetic and calorimetric measurements have been carried out, as well as structural and colloidal characterization of the samples.

We have seen that 35 nm magnetite nanoparticles (see Figure 1) reach the highest heating efficiency of all samples, having a size close to the monodomain-multidomain limit [1]. Additionaly, the heating efficiency of the maghemite nanoparticles grows as the particle size grows [2]. The same behavior has been seen wih the coercive field (see figure 2). On the other hand, analizing samples with the same size and composition but different coatings, no magnetic or calorimetric difference has been found.

All the results obtained from this study are very useful and allow a better understanding of the nanoparticle parameters to achieve an optimized hyperthermia treatment.

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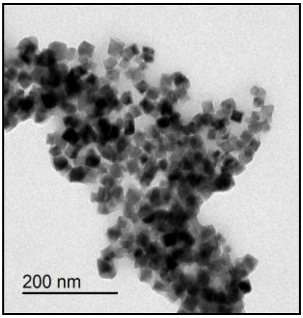

Figure 1: TEM image of 35nm Fe3O4 MNPs.

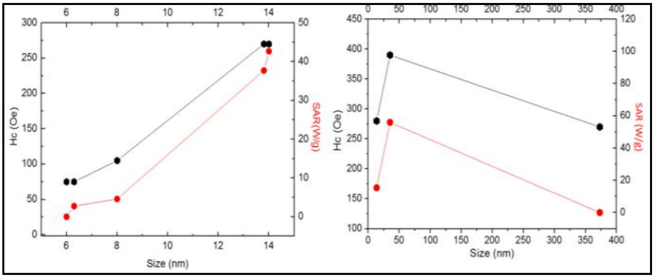

Figure 2: H_C, SAR vs. size. Left: γ-Fe_2O_3. Right: Fe_3O_4. (f=110.5 kHz, 220 Oe).

Simulations of a Planar Silicon Tunnel Field-Effect Transistor

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As planar metal-oxide-semiconductor field-effect transistors (MOSFETs) are scaled to the nanometer regime, their sub-threshold swing (SS) characteristics significantly degrade. This degradation causes a high power consumption limiting the performance of low power transistors in digital applications. Tunnelling-FETs (TFETs) are considered a promising solution to overcome the poor performance of MOSFETs in the sub-threshold region (leakage current (I_{OFF}) and SS) [1] by surpassing the fundamental limit of MOSFETs of 60 mV/dec at room temperature. The on-current (ION) of TFETs depends on the distance between the conduction and valence band because the I_{ON} arises from a band-to-band tunnelling (BTBT) process with low efficiency. Thus the TFETs suffer from a low ION [2]-[3]. In Ref. [3], a new device structure is proposed to overcome the low I_{ON} issue by adding an extra layer between the gate-dielectric and the p-i-n junction in order to increase the tunnelling area. The aim of this work is to investigate and optimise the performance of a TFET based on the experimental device [3]. The n-type Si TFET has a gate length of 1 µm shown in Fig. 1. The epi-layer and the SOI have an intrinsic doping of 1.0×10^{15} cm^{-3}, the p-type source has a concentration of 3.7×10^{19} cm^{-3} and the n-type drain of 2.7×10^{20} cm^{-3}. The work function of the metal gate is 4.8 eV. All the simulations have been performed using Silvaco ATLAS [6] accounting for both the local and non-local BTBT, for the band-gap narrowing, and the thermionic emission transport model. Fig. 2 shows the ID-VG characteristics at a drain bias of 1.0 V comparing simulations with experimental data with a very good agreement at large gate biases. The simulations allow to optimise the device architecture since IOFF increases dramatically with a drain-togate distance (D) while ION shows a minimal change.

Acknowledgment: This work is supported by the Spanish Government and FEDER funds (TEC2014-59402-JIN), by the Spanish Government (TIN2013-41129-P) and also by Xunta de Galicia and FEDER funds (GRC 2014/008).

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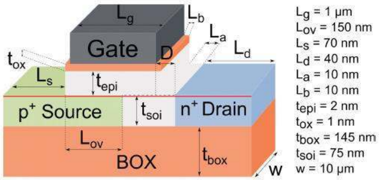

Figure 1: Schematic of the TFET with the corresponding dimensions. The z-direction is assumed to be a 10 µm wide.

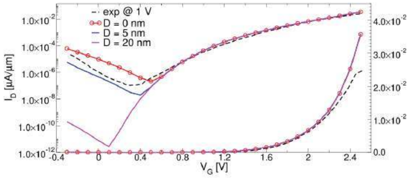

Figure 2: I_D-V_G characteristics on both linear (right) and logarithmic (left) scales at a high drain bias of 1.0 V.

Improve of the paclitaxel activity by the use of polymeric nanoparticles of lactic and glycolic acid: assay in multicellular spheroids from lung cancer cells

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Paclitaxel (PTX) is a cytotoxin used as a drug of choice for the treatment of various types of solid tumors, including breast and lung cancer. However, its commercial formulation (Taxol®) has been associated with several side effects such as hematologic toxicity, bone marrow depression, and painful peripheral neuropathy. In this work, a promising type of polymeric nanoparticles of lactic and glycolic acid loaded with this drug (PLGA-PTX) for the treatment of lung cancer is proposed to solve these limitations. The results of proliferation assays showed significant dose reduction IC50 with PLGA-PTX up to 3.63 and 3.79 times lower in two human lung tumor cell lines A549 and NCI-H460, compared to free PTX. No inhibition was observed in the growth of any cell lines with blank nanoparticles. For cellular uptake studies with fluorescence microscopy, A549 was incubated with Nile red (NR) and NR-loaded NPs at different times. The results obtained suggest that NP-PTX facilitate the incorporation of NR into the cell compared with free NR. Finally, multicellular tumour spheroids (MTS) assays in A549 were performed and MTS were treated with PTX, PLGA-PTX and blank NPs at the IC50 dose of free PTX. MTS growth was monitored with imaging microscopy the apoptosis induced was analyzed by a TUNEL assay. PLGA-PTX caused a significant reduction in the volume of MTS (73%) in comparison to free PTX (46%). In addition, the number of apoptotic cells was higher in MTS treated with PLGA-PTX than in those treated with PTX. The set of results presented in this work suggest that the association of paclitaxel with nanoparticles improves the antitumor effect of the drug and facilitates its incorporation into the tumor cells.

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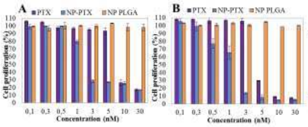

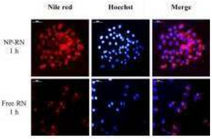

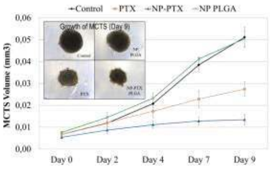

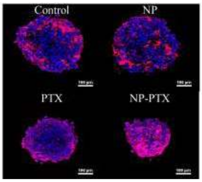

Figure 1: Proliferation assays in A549 (A) and NCI-H460 (B) cell lines. **Figure 2:** Intracellular uptake with RN and NP-loaded RN in A549 cells. **Figure 3:** Analysis of the PLGA-PTX effect in MCTs' growth of A549 cells. **Figure 4:** TUNEL assay in MCTs of A549 cells to detect apoptosis induced (in red).

Surface modification of Nanoporous Alumina towards bio-sensing applications in optical nano-fluidic system

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Abstract

The surface modification of nanoporous anodic alumina (NAA) by grafting functional molecules is a key step in its application as a biosensing probe platform.

Aptamers are single-stranded nucleic acid molecules that bind with high affinity and specificity to their targets. They are a promising class of compounds since their 3D structure leads to bind with a wide variety of biomolecules down to the femtomolar range [1]. In this work we propose and study a path for the atachment of aptamers to NAA based on three steps, as illustrated in Figure 1a. Furthermore, we demonstrate its validity for biosensing based on the reflectance spectroscopy method in a flow cell. The attachment of aptamers is performed in three steps. In the first one, NAA is functionalized by grafting aminopropyl triethoxysilane (APTES) and glutaraldehyde (GTA). This method has already been demonstrated for protein attachment on NAA[2]. Furthermore, it has also been used for DNA attachment to detect ATP [3]. The second step consists of the covalent attachment of streptavidin to the APTES-GTA while the final step is the grafting of the biotinylated aptamer to the streptavidin.

The study of each surface modification step is carried out by FTIR spectroscopy (Figure 1b) where we observe C-H peak of APTES, amide bounds and one broad peak of Streptavidin whose signal intensity depends on the Streptavidin concentration. With experiments by in-situ reflectance spectra monitoring in the flow cell we demonstrate that this surface modification is suitable to use in biosensin probes since when Biotin is injected on the streptavidin-modified NAA signal increase ocur wich mantains when is injected PBS (Figure 1c).

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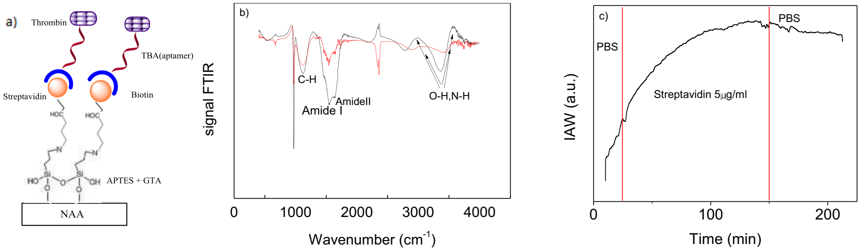

Figure 1: a) Scheme of surface modification b) FTIR spectra with APTES+GTA+ Streptavidin 100μg/ml and 10μg/ml c) Processed reflectance spectra by Average over Wavelength (IAW) of pre-incubated Streptavidin (10 μg/ml) with injection in fluid cell of Biotin (5 μg/ml)

Optimization of protein loading and release based on porous silicon particle size

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Oral administration is contemplated to be the most suitable and comfortable method of delivering drugs because it removes the inconvenience of frequent injections, physical stress, and difficulties in handling proteins. Oral administration of proteins and peptides is limited due to their propensity to degrade in the harsh conditions present in the stomach (i.e low pH, the presence of proteolytic enzymes). Porous silicon is relevant as a drug delivery material because of its biocompatibility, biodegradability, high loading efficiency, and controllable drug release characteristic (hours to months). Porous silicon particles are proven to protect the sensitive cargo from degrading under areas with hostile conditions such as the stomach.

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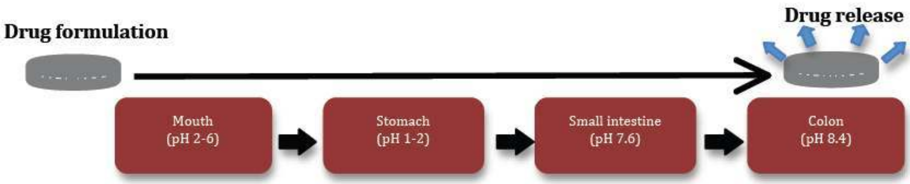

Figure 1: Schematic representation of the body harsh conditons simulated in the experiment.

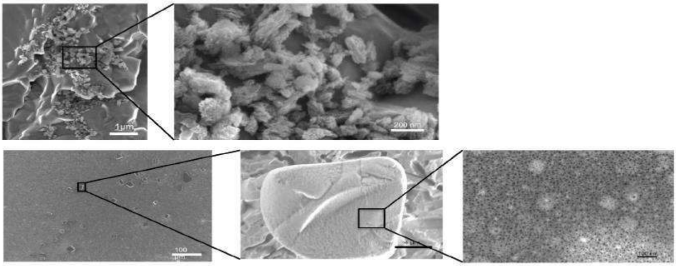

Figure 2: SEM images of the Si particles at diferent magnifications for different particle sizes.

Tripalmitin and p4VP nanoparticles as PTX delivery systems for breast cancer treatment

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Paclitaxel (PTX) is one of the chemotherapics of election for the treatment of breast cancer. However, this drug presents some limitations as low solubility, poor tumor specificity and the appearance of side effects.[1] The use of nanoparticles (NPs) is an asset to improve PTX antitumor efficacy, avoid toxicity and target the drug action specifically on the tumor tissue.[2]

For these reasons, we have developed a delivery sistem, consisting on Tripalmitin solid lipid NPs (Tripalm-NPs) for PTX encapsulation (Tripalm-NPs-PTX). These NPs have been assayed in a wide range of breast tumor models, consisting on a human breast cancer cells (MCF7); multicellular tumor spheroids (MTS) derived from MCF7, that mimick a tumor mass; a resistant cells line through P-glycoprotein (P-gp) overexpression (HCT-15) and breast cancer stem cells (CSCs) obtained from MCF7, which are very often responsible for recurrences and recidives.

In order to asses the antitumor efficacy of these PTX-loaded NPs, treatments were added at increasing concentractions and a cytotoxicity assay was performed by the sulphorrodamine B method after 96 hours. MTS were obtained from MCF7, and their volume after being treated were monitored by microscopy at different times of the experience. Finally, for CSCs obtention, MCF7 were incubated with an induction medium for two weeks, treatments were administered for 48 hours, and the cytotoxicity assay was carried out using a Cell Counting Kit (CCK-8, Dojindo, Japan).

The results obtained prove an improvement in the antitumor efficacy of PTX after its incorporation in Tripalm-NPs-PTX over MCF7 cells and MTS. Further, they were also able to increase PTX effect against a resistant cell line, and CSCs, with a significant ($p<0.001$) decrease in cell viability in all the cases.

According to these results, Tripalm-NPs-PTX are very promising delivery systems to improve breast cancer treatment efficacy and avoid treatment failure.

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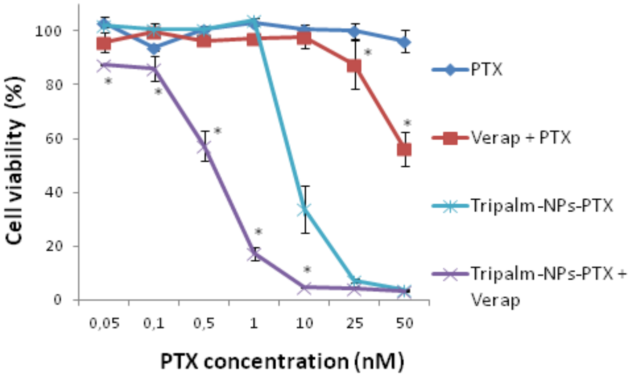

Figure 1: Cell viability (%) of HCT-15 resistant cells after exposure to PTX, Tripalm-NPs-PTX and their combination with verapamil, a P-gp inhibitor. *Significant differences (p<0.001) between treatments with or without verapamil.

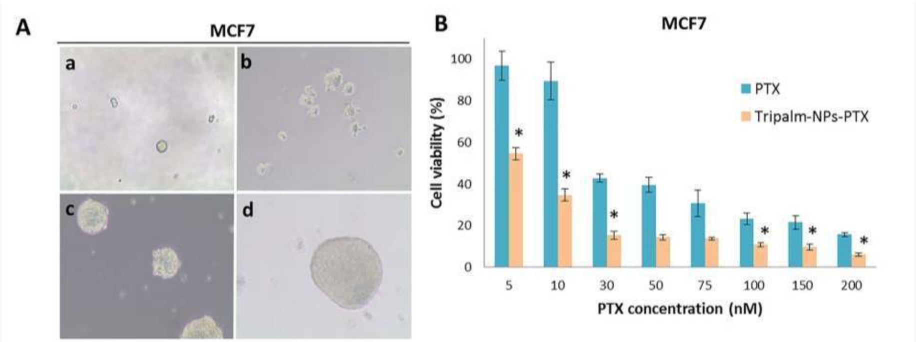

Figure 2: A) Images of breast CSCs after a)1, b)3, c)6, and d)13 days of induction (10x). B)CSCs viability (%) after treatment with increasing concentrations of PTX and Tripalm-NPs-PTX (48 hours). *Significant differences (p<0.001) between both treatments.

Water dispersible silica nanoparticles for biomedical applications

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Abstract

Mesoporous silica nanoparticles are potential agents for biomedical applications. Spherical nanoparticles are synthesized by Stöber method with a core shell structure achieving monodisperse distribution around 50 nm[1] (Figure 1). This work is focused on bioimaging and photodynamic therapy (PDT) applications; for that fluorescent dyes are embedded in the core (bioimaging) and photosensitizers (PS) are grafted on the shell (PDT) functionalized by amine groups (Figure 2).

However, those systems have low stability in water necessary for biomedical applications. In this sense, polyethylene glycol (PEG) is the most used macromolecule to coat the nanoparticles since it is no toxic, biocompatible, it prolongs the nanoparticles life-time in blood, and is approved by the Food And Drug Administration (FDA) for clinical use.[2] PEG of different chain lengths are covalently anchored to external groups (-NH_2 or -OH) of mesoporous silica nanoparticles. A result, silica nanoparticles with dual functionality (imaging and treatment) and well-dispersed in water are achieved. "In vitro" experiments will be carried out to probe their therapy activity in cells.

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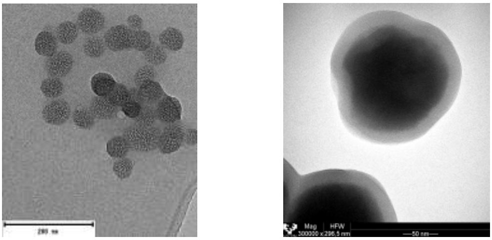

Figure 1: TEM image of mesoporous silica nanoparticles with around 50 nm size (left) and TEM image of the Core-Shell structure of silica nanoparticles (right).

Figure 2: Image of powder synthesized for Rose Bengal grafted onto hydroxyl groups (left) and onto amine groups (right).

Effect of bond tangency/gap on the phase behaviour of athermal polymer packings

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We present results from extensive Monte Carlo simulations on dense and nearly-jammed packings of chains of hard spheres of uniform size [1]. Through a robust chain-connectivity-altering algorithm we are able to simulate chain lengths of 1000 spheres within modest computational time. Local environment and similarity to specific crystal structures are gauged through the crystallographic element norm (CCE) metric [2]. We study the role of bond constraints on the packing efficiency and structural characteristics of polymer assemblies: by increasing the bond tolerance (bond gaps) we observe accelerated crystal nucleation and growth which in turn lead to a wealth of ordered morphologies [3]. In their majority crystals structures with bond gaps are significantly different from the random hexagonal close packing which prevails in the strict tangent limit [4,5]. In general, bond tangency shifts the occurrence of the phase transition to higher packing densities compared to monomers [6] and to chains with bond gaps. Based on these findings using simple geometric arguments we explain the role of rigid and flexible constraints in the phase behavior of general atomic and particulate systems.

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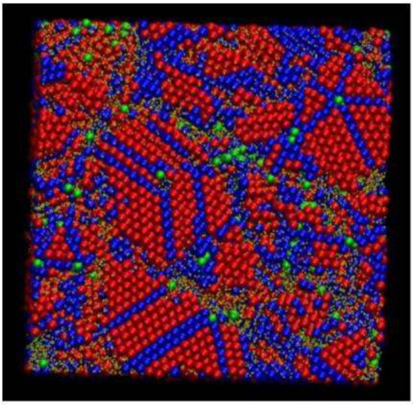

Figure 1: System snapshot of 54-chain hard sphere system of average chain length N = 1000 with bond gaps. Hcp- and fcc-like spheres are shown in blue and red, respectively. Sites with fivefold local symmetry are shown in green.

Using Binary Surfactants to Improve Seedless Synthesis of Gold Nanorods for Use in Cancer Theranostics

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Our group has focussed in recent years on the development of novel nanomaterials and their surface functionalisation for use in cancer theranostics. The synthesis of metal nanoparticles with high absorption in the near-infrared and low quantum yield allows for their application *in-vivo* in photoacoustic imaging and plasmonic photothermal therapy. With recent work including the development of gold nanotubes [1] and hexagonal gold nanoplates [2] for these particular purposes.

We present here a novel seedless synthesis route for gold nanorods (AuNRs) utilising a NaOL-CTAB binary surfactant mixture allowing improved monodispersity, dimensional tunability and shape yield has been developed. The protocol was adapted from the seeded approach previously published by Ye *et al.* [3]. Through variation of the two surfactant concentrations the diameter and length of synthesised AuNRs are controllable over ranges of 10-35 nm and 40-80 nm respectively with a good level of control and reproducibility. Rod shape yields via this protocol are typically in excess of 95%, with yields of 99.99% acheivable at certain morphologies. These particles also demonstrate improved monodispersity compared to other similar CTAB-only based seedless synthesis routes.

These particles have been functionalised through the use of a PSS coating, with individual monomer units replaced with units allow binding of targetting agents to the molecule. These have been tested *in-vitro* with cultured human cancer cells for their toxicological properties and targetting efficacy with promising results. They have also been tested as contrast agents in photoacoustic imaging and as photothermal agents *in-vitro.* Future work will look to extend these models to *in-vivo* models, to demonstrate there efficacy within biological systems.

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Figures

Figure 1: Synthesised AuNR solutions with longitudinal modes between 625nm (left) and 925nm (right). The longitudinal mode increases by 25nm between bottles.

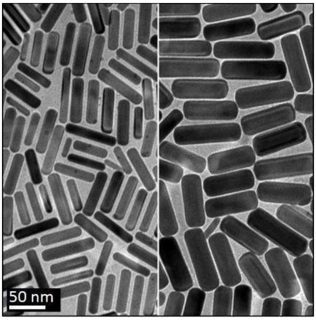

Figure 2: TEM of two batches of gold nanorods synthesized by the above protocol, of average size 12×55 nm (left) and 35×75 nm (right). The scale bar applies to both images.

Macroporous silicon structures in 700 nm and 500 nm

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In this study we report different structures based on macroporous silicon technology. Three photonic crystals of 700 nm pitch with several cavities inserted in the middle structures have been studied (Figure 1). Our work demonstrates that for a single cavity, a peak arises in the middle of the bandgap of the transmission spectrum [1]. However, this peak is not good enough for spectroscopic gas sensing [2]. Introducing more cavities, the quality factor of the peak increses. Futhermore, the bandgap is enlarged and the frequencies inside de bandgap – except in the peaks' area – are more filtered, achieving better optical responses, suitable for spectroscopic gas sensing. On the other hand, we report macroporous silicon pores fabricated in samples with 500 nm pitch. In concrete we present straight and low-modulated pores. Although these structures are simpler than the ones fabricated in 700 nm and they still need to be improved, it is the first time that macropores are successfully grown using the electrochemical etching process at this scale. The aim is to obtain modulated structures able to allow gas sensing in the near infrared range.

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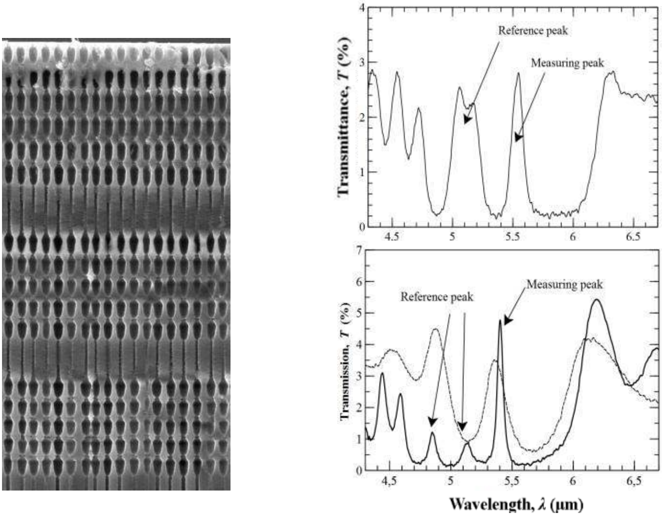

Figure 1: SEM image for a two cavities photonic crystals (left). (Right) Transmission spectra for two (up) and three (down) cavities.

Removal of caffeine and diclofenac from aqueous solutions by adsorption on a multiwall carbon nanotube

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Abstract

Batch sorption experiments were performed to study the adsorption of two emerging pollutants from aqueous solutions using a commercial multiwall carbon nanotube as adsorbent. Caffeine and diclofenac were selected as representative contaminants. The multiwall carbon nanotube from Sigma-Aldrich was characterized by nitrogen adsorption at -196ºC, and through the determination of pHpzc. The effect that several operational parameters, such as initial concentration of organic molecules, mass of adsorbent and contact time, may have on the sorption behavior was also evaluated. The contact time to attain equilibrium for maximum adsorption was found to be 40 min (see Figure 1-A). The kinetic data were fitted to several adsorption models and the adsorption process found to follow pseudo-second-order rate. The equilibrium adsorption data were analyzed using the Freundlich, Langmuir and Toth isotherm equation models (see Figure 1-B).

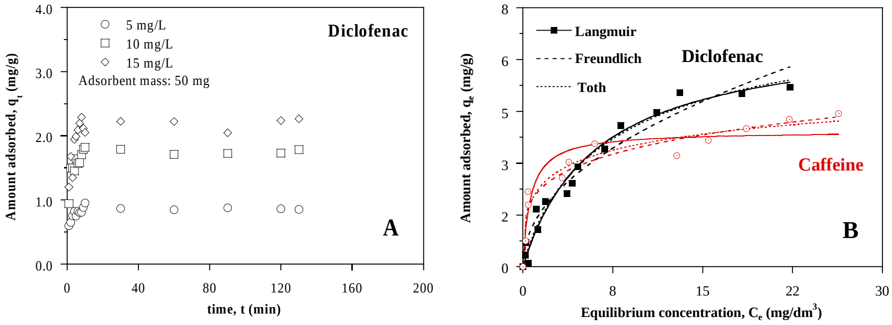

Figure 1: **A**-Kinetic adsorption data for diclofenac on the multiwall carbon nanotube at various concentrations of adsorbate. **B**-Adsorption isotherms for the equilibrium of caffeine and diclofenac on the multiwall carbon nanotube.

Acknowledgements

The authors thank financial support from the Spanish Ministry of Economy, Industry and Competitiveness (MINECO) through the project MAT2013-47811-C2-1-R.

Magnetic and chemical propulsion of mesoporous nanorods as nanomotors

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The research in nanomotors and nanomachines has attracted increasing interests during the last years due to the applicability of these kinds of structures in different fields (biomedicine, energy, catalysis, nanoengineering). In this line, the synthesis of new micro and nano-structures which could be propelled by means of different actuation forces is of great interest in the nanomotors field. In our laboratory, a new methodology has been developed to electrochemically grow mesoporous metallic nanorods (NRs) [1, 2]. In the present work we study the movement of two types of magnetic mesoporous NRs (CoNi and CoNi@Pt) under two actuation forces: oscillating magnetic fields at different frequencies and field strenghts, and chemical forces generated by a gas during a chemical reaction.

Both kind of synthesised mesoporous NRs respond to rotatory magnetic fields giving to a continuous rolling movement and in the direction defined by the field (Figure 1a). When borohydride is present in the aqueous solution, the CoNi@Pt NRs show a stepped rolling movement. It can be explained by the hydrogen generated during NRs catalyzed borohydride decomposition. The massive exit of the H_2 gas entrapped into the nanorods'pores togheter with the magnetic field propel de NRs in a stepped trajectory (Figure 1b). CoNi NRs are poor catalysts to borohydride decomposition and only the magnetic force significantly affects their displacement.

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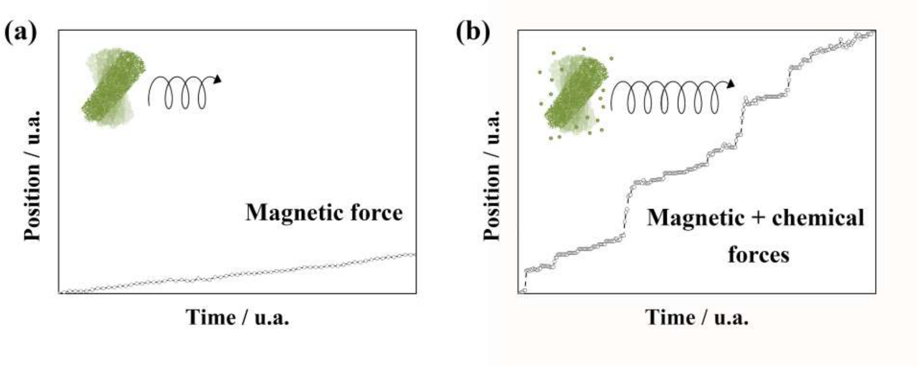

Figure 1: Trajectory of CoNi@Pt NRs in (a) aqueous media and (b) sodium borohydride solution.

Spectroscopic Studies of Molecular Arrangements in Photoreactive Liquid Crystal Mixtures

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The use of photo-reactive liquid crystals (LC) with acrylate functional groups, i.e. reactive mesogen molecules, has shown to be one of promising ways of constructing ultra-thin and high quality optical retardation films. It has been known that the orientation status of LC molecules during a curing process may affect the molecular arrangement in the cured film, and thus determinng physical and optical properties of the film [1-3]. In the present study, spectrocopic techniques were employed to investigate curing and alignment mechanisms of LC molecules on various processing conditions. The miscibility of LC molecules with non-reactive rigid molecules have been studied using FTIR and Raman spectroscopic methods. DSC experiments were conducted to investigate the thermodynamic behavior of mixed liquid crystals. Polarized FTIR and UV/Vis spectroscopy were used to study the change in the molecular orientation of photo-reactive mesogen molecules before and after photo-curing reactions.

Mixtures of a reactive mesogen with a small size liquid crystal exhibit a depression of transition temperature from LC to liquid phase. Since small LC molecules impede the formation of regular arrangement of reactive mesogen molecules, they behave like impurities which retard the formation of the LC phase. By curing the LC mixture, which shows a uniform nematic LC phase, a network structure is formed with the reactive mesogen, and the arrangement of LC molecules are maintained over the transition temperature from LC to liquid phase. The small LC molecules in the LC mixture maintain the same molecular arrangement with the reactive mesogen molecule through π-π interactions.

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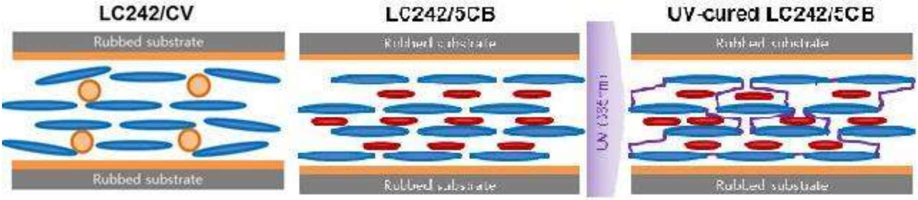

Figure 1: Various models of the molecular arrangement of nematic liquid crystal mixtures.

Magnetic Domains in CoCrPt films with Perpendicular Magnetic Anisotrpy

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CoCrPt alloy thin films, with strong uniaxial magnetocrystaline anisotropy, have been studied for the design and development of perpendicular magnetic recording media. The nanoscale patterning of these films has also been considered of great interest in patterned magnetic recording media, as well as for sensors and logic devices applications. [1,2] In this work, we study the magnetic domain dynamics of continuous and patterned CoCrPt films. An Interference Lithography (IL) system has been used to design pattern templates on silicon wafers. A 5 nm seed layer of Ti followed by 10 nm of CoCrPt and 3 nm Ti capping layer were deposited on the templates using an RF sputtering system at room temperature. Lines and dots patterns with periodicities ranging from 1000 to 700 nm and features sizes from 400 to 800 nm were fabricated. Magnetic characterization was performed using a vibrating sample magnetometer (VSM) and a magneto-optical Kerr (MOKE) microscope. An atomic force microscope (AFM) was used for topographic characterization. Magnetic domains in CoCrPt film nucleate and grow with the external field resembling a fractal structure. However, the reversal of patterned CoCrPt films follows a different mechanism due to confinement effects. This work was supported by grants: EU FP7-IRSES-318901, Spanish MINECO FIS2013-45469 and FIS2016-76058

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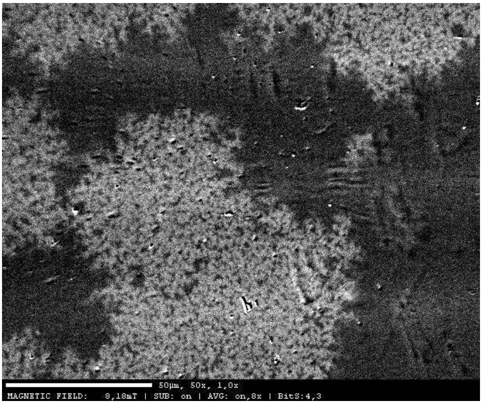

Figure 1: MOKE image of magnetic domains in a 10 nm CoCrPt film.

Gold Loaded Thermoresponsive Nanogels with Multiple-Associated Anti-Tumour Effects

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Most chemotherapeutic treatments include combination therapy to inhibit tumour growth, yet the systemic method of administration involving separate drug formulations results in undesirable side effects with a complicated dosing strategy. Consequently, the ability to combine multiple drugs in a single nanoparticulate delivery system is of interest. In this context, we have explored thermosensitive nanogels based on polyethylene glycol methacrylate decorated with gold nanoparticles (AuNPs) for their ability to deliver drugs upon external stimuli. Within these vehicles we include two drugs of interest for tumour treatment, doxorubicin and pomalidomide. The biological effects of doxorubicin are well documented whereas pomalidomide remains a relatively novel drug that has shown promising results in the treatment of multiple myeloma (MM), among other actions including the inhibition of angiogenesis and anti-inflammatory cytokines secretion. *In vitro* experiments were conducted to assess the cytotoxic and anti-angiogenic effects of released doxorubicin and pomalidomide respectively. Additionally we investigated the ability of external stimuli and the usage of near infrared light as trigger for combinationtherapy and hyperthermia. We further demonstrate that an additional polymer coating on the nanogel surface can decrease uncontrolled drug leakage, and modulate cellular uptake and drug release profiles.

An approach to assess and control the potential risks related to nanomaterials- the case of INSPIRED project

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Abstract

The use of engineered nanomaterials in a wide number of consumer, medical and industrial applications has led to increase the interest to understand potential safety issue derived from the use of these new materials. To guarantee the implementation and the social acceptance of the nano-based products/processes it is necessary to ensure that they do not pose an additional risk for health or the environment.

The INSPIRED project [1] (Grant Agreement No 646155; 2015-2018) deals with the use of engineered nanomaterials for printed electronic applications. Its goal is to scale-up the whole value chain to ensure the availability of nano-based functionalised inks in industrial scale quantities and enable rapid high-throughput production of novel printed electronic components on a wide variety of substrates. INSPIRED runs in parallel the development of the pilot production lines and the assessment of potential impacts from nanomaterials (nanosafety assessment). Specifically, the focus of these activities is the identification, evaluation and control of potential environmental and worker exposures to avoid related risks. The approach includes the use of state-of-the-art qualitative and semi-quantitative risk assessment tools as ECETOC TRA [2], Stoffenmanager-Nano [3] and ISO 12901-2 [4] to identify “hot-spots” in the process and to rank possible risks derived from the use of the engineered nanomaterials. For selected scenarios, quantitative measures may be performed to assess the potential release of nanoparticles and to check the efficiency of controls to reduce worker exposure (following the harmonized tiered approach from the OECD, 2015 [5]). The final goal of this approach is to develop guidance to achieve safe nano-related processes that may foster the development of printed electronic applications.

This project has received funding from the European Union’s Horizon 2020 research and innovation program under grant agreement No 646155.

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Multisegmented Ni/Au Nanowires: Electrosynthesis, Characterization, Magnetic Locomotion, and Functionalization

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Micro- and nanotechnologies are currently playing an important role in the development of novel biological nanoscale diagnostic and drug-delivery tools, thanks to significant advances in micro- and nano-structured materials [1]. In this regard, electrodeposition is an efficient technology for micro- and nano-fabrication, especially the template-assisted electrodeposition of metals and alloys. Such a template-assisted electrodeposition route allows a reproducible preparation of nanowires of different sizes and compositions. Currently, with multisegment nanowires based on different materials, electrosynthesis is a focus of great interest as a consequence of their multicomponent architecture that allows the integration of various functions (e.g., locomotion, drug retention, and recognition) that can enhance the efficacy of these biological tools [2].

Here, we propose a facile fabrication pathway for the synthesis of magnetic multisegmented nanowires of Ni and Au (100 nm in diameter and approximately 2 µm in length) to be used as nanocarriers; this combines two different functionalities as a consequence of the two different surfaces (Au and Ni) and, moreover, by means of the action of an external magnetic field, facilitates their movement, directionality, and efficacy. This research consists of creating highly sophisticated multifunctional systems from ecologically friendly formulations for the development of highly biocompatible materials with enhanced efficiency.

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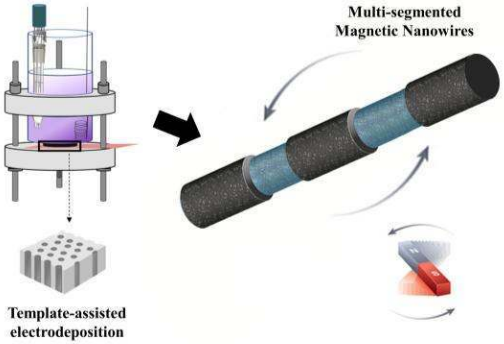

Figure 1: Schematic representation of magnetic multisegmented nanowires of Ni and Au

Non-conventional covalent modification of graphene under microwave conditions

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Graphene is a promising next-generation material with a unique set of electronic, mechanical, and thermal properties. Consequently, graphene exhibits a wide variety of potential applications in the field of biomedicine such as sensing, bioelectronics, implants and drug delivery.[1] Besides, chemical functionalization of graphene is a topic of paramount importance, because it allows the fine-tuning of material's chemical and physical properties.[2] Surface modification of graphene frequently requires tedious and long procedures. However, the use of non-conventional conditions reduces timing, avoids unstable suspensions and improves the reaction efficiency.[3]

This project is focused on relatively unexplored cycloaddition reactions of arynes with exfoliated graphene. In particular, we generated different arynes by thermal decomposition of the corresponding aryl anhydride at high temperatures by microwave irradiation using solvent-free conditions (Figure 1). Graphene played two roles in this reaction process: as reagent and as microwave absorbing matrix.

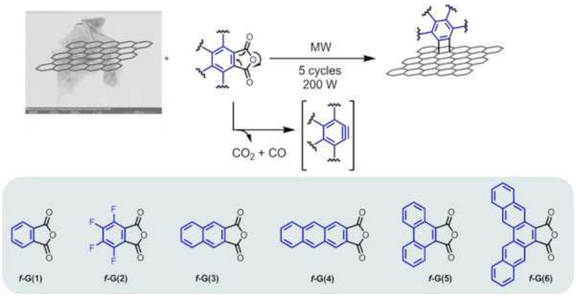

Figure 1: Schematic representation of the chemical modification of graphene.

In conclusion, we have developed effective and controlled methods to functionalize different graphene derivatives, in order to modulate their properties and to specifically adequate the material as a component for new medical devices in the future.[4]

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Mechanical properties of nanocomposite Mo_2BC nanolaminates

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State-of-art ceramic protective coatings such as TiN, TiAlN, c-BN etc. generally exhibit high hardness and stiffness. However, these positive features are often accompanied with brittle deformation behavior. To overcome this limitation a new type of material combining high hardness with moderate ductility is desired. Recently, there has been an increased interest in Mo_2BC nanolaminates which favorably combine the properties attributed to ceramics and metals [1,2].

For the preparation process the co-sputtering of C, Mo and B4C targets was used and the deposition was carried out on hardmetal, steel and silicon substrates. Mid-frequency pulsed DC plasma excitation was used to enhance the ion flux on the substrate and consequently to enhance the crystallization. The hardness and elastic modulus were measured and evaluated by depth sensing nanoindentation, the resistance to cracking was evaluated by scanning electron microscope of the residual imprints made by indentation. The above mentioned deposition conditions resulted in partially crystalline nanocomposite coatings with ~2 nm sized Mo_2BC grains embedded in an amorphous matrix. The analysis of mechanical properties proved the presence of superior fracture toughness combined with high hardness of about 27 GPa and low surface roughness. The further thermal annealing improved both the hardness (increased to 32 GPa) and elastic modulus due to the enhanced crystallization of the Mo_2C and Mo_2BC phases to the detriment of the amorphous phase; however, the fracture toughness decreased.

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Figures

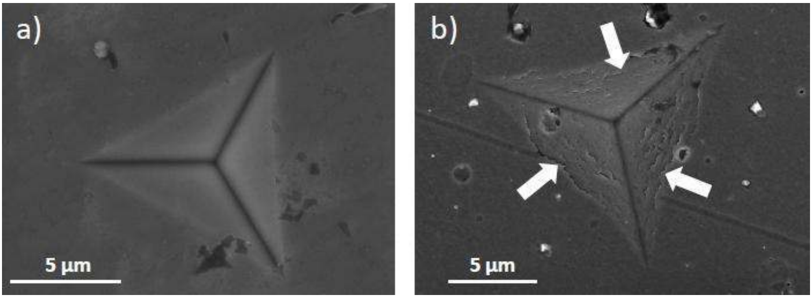

Figure 1: a) The residual imprint in the Mo_2BC coating (hardness 26 GPa) made by indentation using 1 N load and b) the residual imprint in TiAlN coating (hardness 25 GPa) with marked picture frame cracks.

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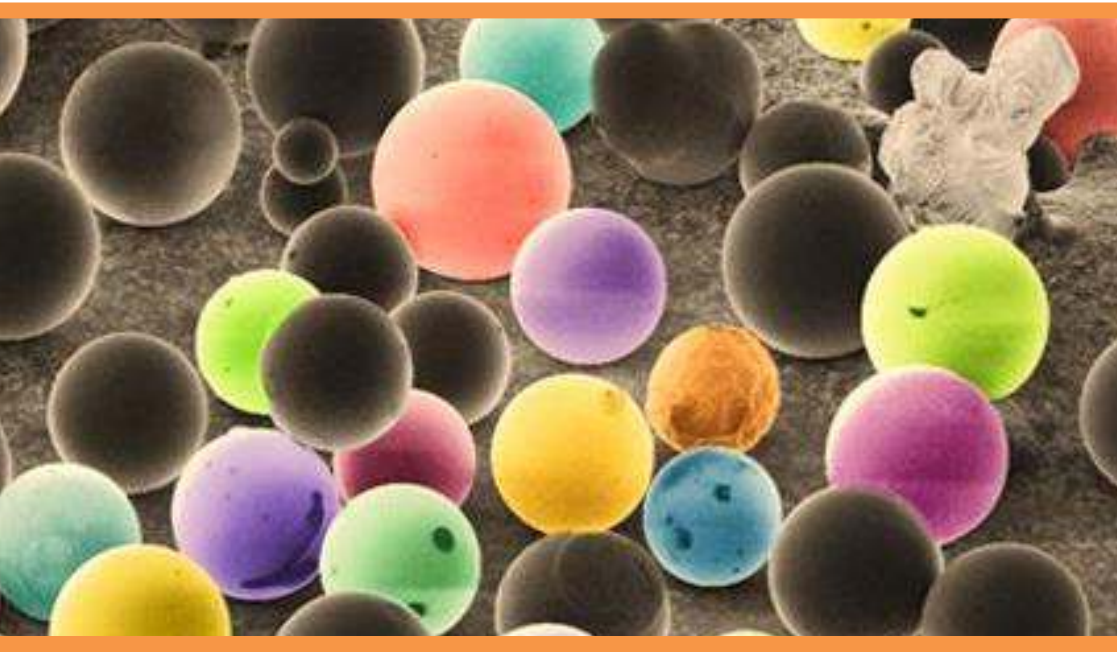

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