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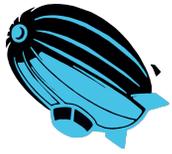
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ABSTRACTS BOOK

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On behalf of the Organising Committee we take great pleasure in welcoming you for the first edition of **ImagineNano** Online (September 29-October 01, 2020).

Due to the current COVID-19 situation worldwide, organisers decided to postpone the in-person edition to 2021 and merge 3 events (nanoSpain / graphIn / 3PM) to propose a 3-days online International Conference (IM2020 Online). This event will present the most recent advances in fundamental research & technology developments in Nanoscience and Nanotechnology (N&N). 33 high profile talks from worldwide most influential academia/industry experts in the N&N sector will present speeches in this international event on how advanced materials will change the future of technology and impact positively our daily life in sectors such as Energy, Electronics or Biohealth.

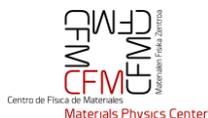
We would like to thank all speakers and participants that joined us this year for this online edition.

Hope to see you again in the next in-person edition of **ImagineNano** (May 25-27, 2021) in Bilbao (Spain).

● ORGANISER



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Graphene Nanoelectronics at the Edge

Walt A de Heer

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From the start of graphene electronics research, the primary goal has been to succeed silicon and to develop a graphene platform for 21st century nanoelectronics, analogous to the transition from vacuum tubes to solid state electronics. This requires a graphene platform that is compatible with large scale nanoelectronics processing, and a new electronics paradigm. The pioneering Georgia Tech epigraphene electronics program established 2001 [1] was based on this principle. Originally funded by Intel, it has since produced numerous important breakthroughs [2] including a demonstration of large scale device production [3], and the discovery of elusive edge state with extraordinary electronic properties [4], predicted decades ago. Epigraphene, is graphene that is grown epitaxially on silicon carbide (SiC) crystals. The edge state is a unique coherent 1D topologically protected electronic mode involving both edges of graphene ribbons. It is observed in lithographically patterned, non-polar epigraphene but not in deposited graphene because of pervasive edge disorder. In this talk I will present an overview of the epigraphene program and very recent developments on conventionally patterned epigraphene showing that:

- The transport in graphene ribbons is dominated by the 1D ballistic edge state whose conductance is $1 e^2/h$.
- Mean free paths exceed 40 μm even at room temperature, more than 1000 times greater than the 2D bulk.
- The edge state appears to be spin polarized.
- Branched gated edge state networks can be patterned for quasi 1D coherent ballistic nanoelectronics.

Epigraphene is currently the only graphene nanoelectronics platform that is at the edge of being realized. Coherent graphene nanoelectronics has become a distinct possibility.

References

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- [2] C. Berger *et al*, Epigraphene: epitaxial graphene on silicon carbide; Landolt-Börnstein New Series, Subvolume III/45B, hal-01513323 (2017).
- [3] M Sprinkle, *et al* Scalable templated growth of graphene nanoribbons on SiC *Nature nanotechnology* 5 (10), 727-731 (2010)
- [4] J. Baringhaus *et al*, Exceptional ballistic transport in epitaxial graphene nanoribbons, *Nature* volume 506, pages349–354(2014)

● KEYNOTES

Nano-optics in 2D materials

Pablo Alonso-González

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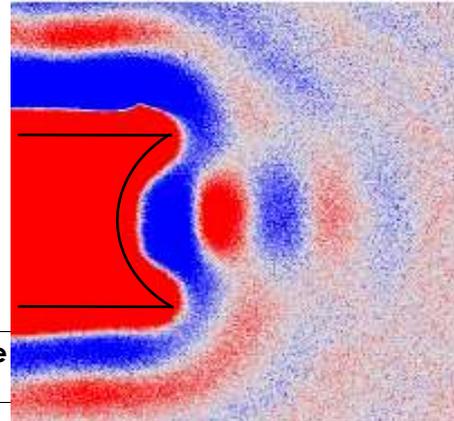
Abstract

The advent of two-dimensional (2D) materials and their extraordinary optical properties has allowed the visualization of nanolight in the form of electrically tunable (active) plasmon polaritons in graphene¹ or low-loss phonon polaritons in h-BN² or α -MoO₃³ thus introducing a very encouraging arena for scientifically ground-breaking discoveries in nano-optics. In this talk I will show our latest studies on the tunability and manipulation of phonon polaritons in hyperbolic van der Waals crystals, which allow for controlling light at the nanoscale (nano-optics) with unprecedented capabilities.

References

- [1] Chen, J. et al. Optical nano-imaging of gate-tunable graphene plasmons. *Nature* 487, 77 (2012).
- [2] Dai, S. et al. Tunable Phonon Polaritons in Atomically Thin van der Waals Crystals of Boron Nitride. *Science* 343, 1125-1129 (2014).
- [3] Ma, W. et al. In-plane anisotropic and ultra-low-loss polaritons in a natural van der Waals crystal. *Nature* 562, 557–562 (2018).

Figures



Figure

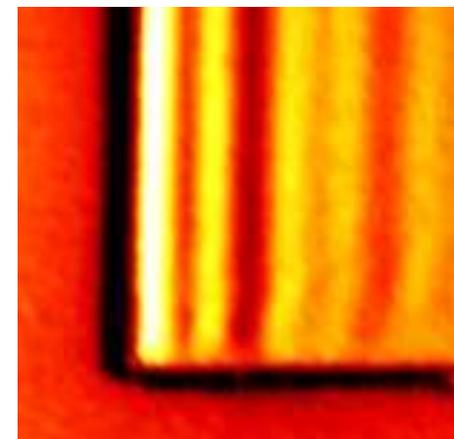


Figure 2: Anisotropic propagation of phonon polaritons in α -MoO₃

4D transmission electron microscopy: imaging soft materials and biologicals in liquid phase

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Water is a critical component for both function and structure of soft matter and it is what bestows the adjective soft. Imaging samples in liquid state is thus paramount to gathering structural and dynamical information of any soft materials. Herein we propose the use of liquid phase electron microscopy to expand ultrastructural analysis into dynamical investigations. We imaged several soft materials including vesicles, micelles, gels as well as several proteins in liquid phase using transmission electron microscopy and demonstrate that the inherent Brownian motion associated with the liquid state can be exploited to gather three-dimensional information of the materials in their natural state. We call such an approach Brownian tomography (BT). We combine BT with single particle analysis (Brownian particle analysis BPA) to image protein structures with a spatial resolution close that achievable using cryogenic TEM. We show that BPA allows sub-nanometre resolution of soft materials and enables to gather information on conformational changes, hydration dynamics, and the effect of thermal fluctuations.

Relevant references:

G. Marchello, C. De Pace, A. Duro-Castano, G. Battaglia, and L. Ruiz-Perez End-to-end image analysis pipeline for liquid-phase electron microscopy *Journal of Microscopy*, Vol. 279, Issue 3 2020, pp. 242–248
G. Marchello, C. De Pace, N. Wilkinson, L. Ruiz-Perez, G. Battaglia *arXiv* preprint arXiv:1907.03348

Blind ghost imaging through scattering media

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The propagation of coherent light through a scattering medium produces speckle patterns in reflection and transmission. Despite the apparent randomness of the speckle patterns, a spatial correlation between the reflected and transmitted intensities survives even in the multiple scattering regime [1]. The existence of mutual information between the two sides of a scattering medium opens up new possibilities for the control of light transmission, and for sensing and imaging [2]. Here we show that ghost imaging can be performed to image a target located behind an opaque scattering layer, without measuring the transmitted speckle [3].

References

- [1] I. Starshynov, A.M. Panagua-Diaz, N. Fayard, A. Goetschy, R. Pierrat, R. Carminati, J. Bertolotti, *Phys. Rev. X* **8** (2018) 021041.
- [2] N. Fayard, A. Goetschy, R. Pierrat, R. Carminati, *Phys. Rev. Lett.* **120** (2018) 073901.
- [3] A.M. Panagua-Diaz, I. Starshynov, N. Fayard, A. Goetschy, R. Pierrat, R. Carminati, J. Bertolotti, *Optica* **6** (2019)460.

Figures

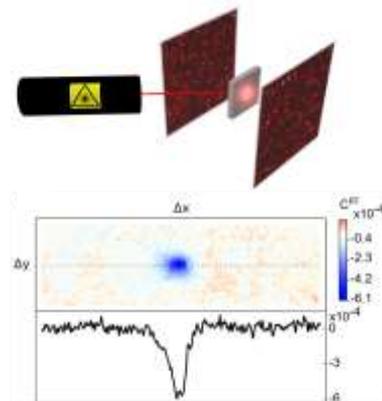


Figure 1: Top: reflected and transmitted speckle patterns measured on both sides of an opaque scattering layer. Bottom: reflection-transmission intensity correlation function. Adapted from [1].

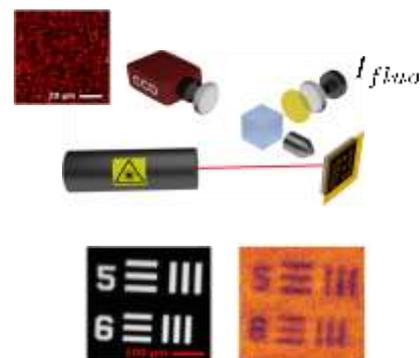


Figure 2: Top: scheme for blind ghost imaging. The object is placed behind an opaque scattering layer, and deposited on a fluorescent substrate. An image is reconstructed from the reflected speckle pattern measured on a CCD camera, and the backscattered fluorescent intensity. Bottom: object and reconstructed image. Adapted from [3].

Van der Waals Contacts on 2D Semiconductors

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Abstract

Ultra-clean van der Waals interfaces can be achieved between soft indium metal and monolayer 2D transition metal dichalcogenide semiconductors. Such interfaces lead to low contact resistance and n-type field effect transistors with high mobilities – in excess of $100 \text{ cm}^2\text{-V}^{-1}\text{-s}^{-1}$. It has been, however, challenging to make similarly clean interfaces between refractory metals with high work functions to achieve efficient hole injection. Here, I will present our efforts on realizing p-type contacts using high work function metals and alloys. We show that it is possible to deposit a thin layer of indium and then a high work function metal on top of it to form an alloy by annealing at 200°C . This method preserves the ultra-clean interface between the monolayer semiconductor and alloy while increasing the work function so that p-type devices can be realized. We also demonstrate clean interfaces using metals such as Au and Pt via direct deposition. These interfaces reveal low contact resistance and also high mobility p-type devices.

References

- [1] Y Wang, J C Kim, R J Wu, J Martinez, X Song, J Yang, F Zhao, A Mkhoyan, H Y Jeong, M Chhowalla, Nature (2019) 568, 70 – 74.

Figures

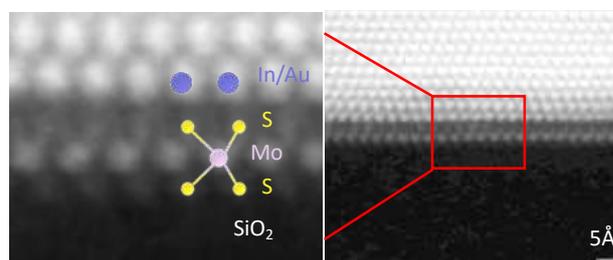


Figure 1: High resolution cross-sectional TEM image of the interface between 3D metal and 2D MoS₂ semiconductor.

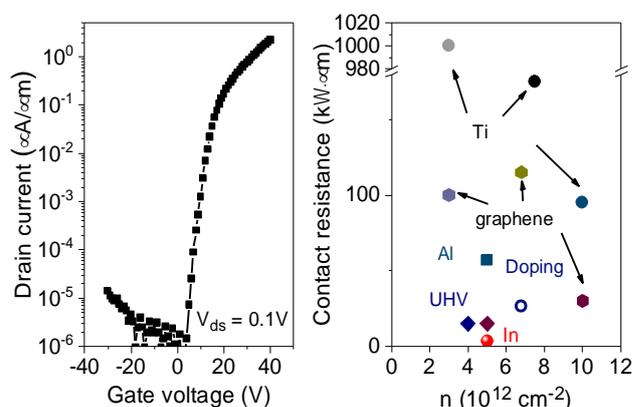


Figure 2: Left: Transfer characteristics of single layer MoS₂ FET with van der Waals contacts showing a mobility of $\sim 170 \text{ cm}^2\text{-V}^{-1}\text{-s}^{-1}$. Right: Comparison of contact resistance of different electrode materials and Indium.

Pinning Effects at Hybrid Interfaces : A Theoretical Insight

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Molecules covalently attached to substrates play a pivotal role in nanoelectronics, in particular for the development of smart surfaces or molecular junctions. The energy level alignment between the molecular levels and the density of states of the substrate dictates the electronic properties of self-assembled monolayers and the amplitude of the current flowing across junctions. The molecular levels are typically broadened upon adsorption and shifted in energies due to interfacial charge redistribution processes. The conventional wisdom suggests that the alignment can be fine tuned by adding electroactive substituents on a given molecular backbone or by increasing the size of the conjugated path. However, several of our recent theoretical studies have evidenced strong pinning effects implying that the alignment can be insensitive to such chemical derivatizations. This has strong implications in many research areas since any molecular design performed in solution can be ruined when attaching molecules to the substrate. In this presentation, we will illustrate such pinning effects in several situations : (i) dye adsorbed on a TiO₂ substrate in the field of dye-sensitized solar cells [1]; (ii) conjugated backbones of increasing size or with different substituents attached to a gold electrode [2,3]; and (iii) photochromic molecules inserted into molecular junctions [4,5].

References

[1] I. Arbouch et al. *Physical Chemistry Chemical Physics* **19** (2017) 29389-29401.

[2] V. Diez-Cabanes et al *Advanced Theory and Simulations* **1** (2018) 1700020.

[3] S. Rodriguez-Gonzalez et al. *Journal of Physical Chemistry Letters* **9** (2018) 2394-2403.

[4] C.Van Dyck et al. *Physical Chemistry Chemical Physics* **15** (2013) 4392-4404.

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Figure

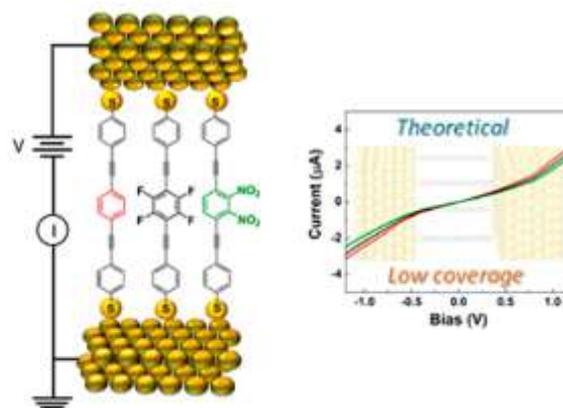


Figure 1: Illustration of the pinning effects in molecular junctions

Networks of two-dimensional materials for electronic applications

Gianluca Fiori

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Two-dimensional materials are considered as potential candidates for flexible electronic applications, due to their outstanding electrical and mechanical properties shown so far.

In particular, devices fabricated through printed techniques can be an intriguing option, where networks of flakes could represent the constituting layers of the devices such as the channel, the dielectric and the contacts.

The physics behind is however far from being understood so that numerical simulations based on a multi-scale approach could represent the only tool in order to shed a light on the main mechanisms at play.

In this talk, we will provide a detailed analysis of the performance to be expected in printed devices through numerical simulations.

At the same time, we will also present an overview of experimental results based on networks of two-dimensional materials.

Figures

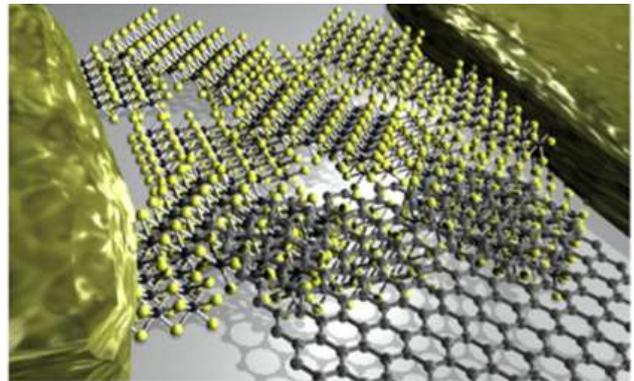
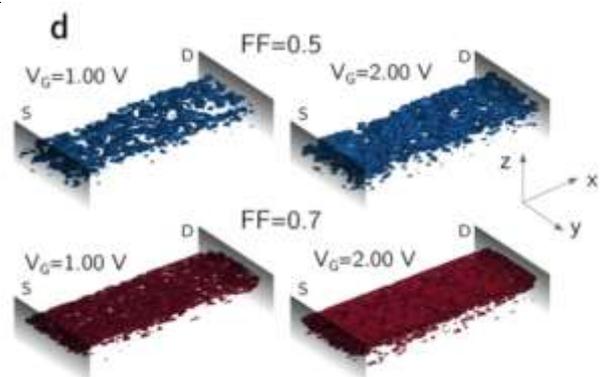


Figure 1: Networks of two-dimensional materials between two metallic gates

Figure 2: Simulated charge transport in a network of flakes for different applied biases



Control of Light at the Atomic Scale: Fundamentals and Applications

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Two-dimensional materials have been recently shown to host robust polaritonic modes, ranging from plasmons in highly doped graphene to excitations in transition metal dichalcogenides. The electromagnetic behavior of these modes can be well understood in terms of an effective surface conductivity, in which we can capture their strong dependence on temperature and external static electric and magnetic fields. Recent advances have also been produced in the synthesis of thin noble-metal films, which open new possibilities for exploring entirely new regimes of nanometallic plasmonics. In this talk, I will overview the general characteristics of the optical response of these materials, which we can understand in terms of simple theoretical descriptions. We will also cover more sophisticated descriptions, aiming at exploring genuinely quantum-mechanical effects. We will further overview recent advances in ultrafast optical response and nonlinear optics, as well as the potential application of these materials for light modulation, quantum-optics, and optical sensing.

This work has been supported in part by the Spanish MINECO (MAT2017-88492- R and SEV2015-0522), the ERC (Advanced Grant 789104- eNANO), the Catalan CERCA Program, and Fundació Privada Cellex.

Extraordinarily transparent compact metallic metamaterials

Vincenzo Giannini

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Metals are highly opaque, yet we show numerically and experimentally that densely packed arrays of metallic nanoparticles can be more transparent to infrared radiation than dielectrics such as germanium, even for arrays that are over 75% metal by volume. Despite strong interactions between the metallic particles, these arrays form effective dielectrics that are virtually dispersion-free, making possible the design of optical components that are achromatic over ultra-broadband ranges of wavelengths from a few microns up to millimetres or more.

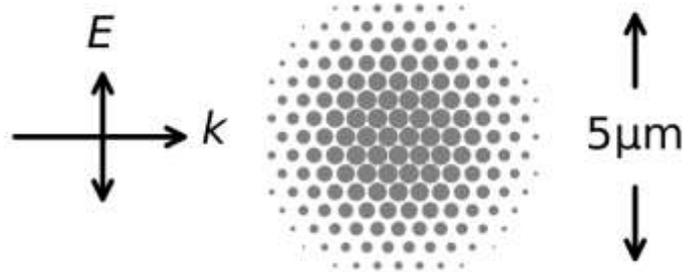
Furthermore, the local refractive indices may be tuned by altering the size, shape, and spacing of the nanoparticles, allowing the

design of gradient-index lenses that guide and focus light on the microscale (see figure 1). The electric field is also strongly concentrated in the gaps between the metallic nanoparticles, and the simultaneous focusing and squeezing of the electric field produces strong 'doubly-enhanced' hotspots (see figure 2)

which could boost measurements made using infrared spectroscopy and other non-linear processes over a broad range of frequencies, with minimal heat production.

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Figures

Figure 1: Schematic of a 'concentrator' gradient-index lens composed of gold nanocylinders on a triangular lattice with 50nm site-to-site separation

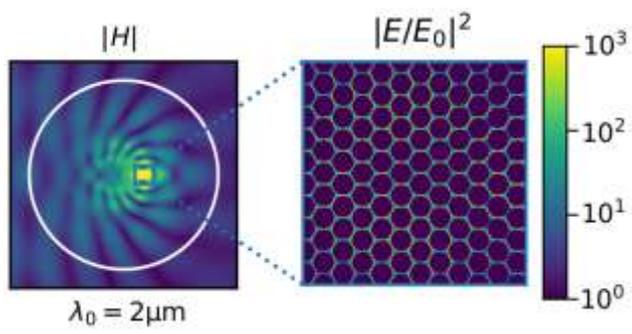


Figure 2: Magnetic near-fields and broadband 'doubly-enhanced' electric field hotspots

Nanomaterials for Emerging Photovoltaics: Halide Perovskite Solar Cells

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Abstract

Halide perovskite solar cells (PSCs) have revolutionized the photovoltaic arena providing power conversion efficiencies currently above 25 %, low cost and ease of fabrication. Their low-weight, semi-transparency and flexibility make them ideal energy sources for applications in self-powered devices required for the future internet of things (IoT). Their combination in tandem architectures with Silicon solar cells will permit building a terawatt-scale energy production required for low-carbon economy, shaping the energy future of our society. In this talk we will present our most recent development related to the synthesis and application of nanostructured materials applied in perovskite solar cell as transport layers and as absorbers. We will demonstrate the importance of the use of organic additives for the passivation of defects increasing devices efficiency and lifetime. We will also show how nanomaterials can be synthesized at low temperature to be compatible with the printing processing methodologies required for the fabrication of printed solar cells. We will show the fabrication of highly stable and highly efficient PSCs that can last more

than 1000 h under continuous irradiation retaining their initial efficiency of 21 %. We will also show the application of semiconductor oxides as transport layers in PSC (Figure 1).

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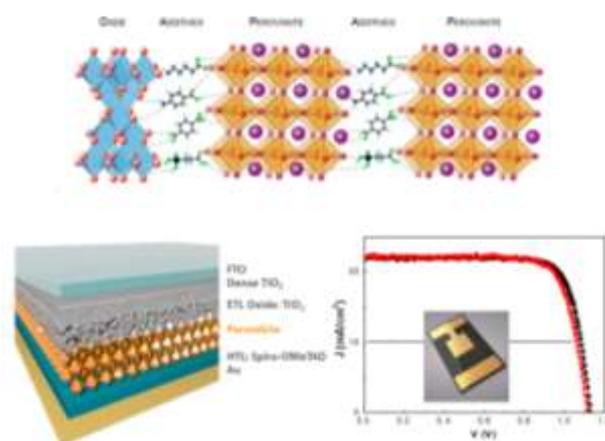


Figure 1: Halide perovskite solar cells. Interaction between transport layers such as oxides, the halide perovskite and different organic additives (top). Schematic representation of a Perovskite solar cell (bottom left) and an IV curve and an image of a device analysed under 1 sun (bottom right).

Self-Assembly of Plasmonic Nanoparticles Under Confinement

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Abstract (Century Gothic 11)

Self-assembly of nanoparticles comprises spontaneous organization of the building blocks into ordered structures by thermodynamic and other constraints. Among other potential forces driving self-assembly, hydrophobic interactions are non-specific interactions, emerging when water molecules rearrange as two hydrophobic species come close to each other. Prediction of hydrophobic interactions at the level of nanoparticles (Brownian objects) remains challenging, because of uncontrolled diffusive motion of the particles. We have developed a general methodology for solvent-induced, reversible self-assembly of gold nanoparticles into 3D clusters with well-controlled sizes. Theoretical description of the process confirms that hydrophobic interactions are the main driving force behind nanoparticle aggregation. Even though self-assembly is then reversible, a limiting factor in this process is the need for constant sample dilution in assembly/disassembly cycles. Changes in nanoparticle concentration alter the kinetics of the subsequent assembly process, limiting optical signal recovery. This problem can be solved by confining hydrophobic nanoparticles within permeable silica nanocapsules, so that the number of nanoparticles participating in cyclic aggregation remains constant, despite of bulk changes in the solution. When this process is applied to plasmonic nanoparticles, highly reproducible plasmon

band shifts are obtained at different solvent compositions.

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Is it worth collapsing a polymer chain? *In vitro* biocompatibility and *in vivo* distribution studies of Dextran based SCPNs and non-crosslinked polymer

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Introduction

SCPNs are soft nano-objects obtained by controlled compaction of a unique chain of the polymeric precursor. In spite of the progress in terms of synthesis and characterization and the promising scenery for future applications in biomedicine, there are no examples of SCPN-based nanomedicines at present.

Here, a validated *in vitro* model of the human airway epithelium and *in vivo* SPECT lung imaging were carried out to demonstrate the advantages of SCPN compared to the corresponding non-crosslinked polymer.

Results and Discussions

After demonstrating the cytocompatibility of both DXT-SCPNs and DXT, cellular uptake of both compounds was studied at 2 concentrations. Regardless of the concentration, DXT-SCPNs showed a faster internalization in both cell types. This effect was more evident in the case of BEAS2b cells, where only 1 hr was required for >90% of the cells incubated with the NPs at of 0.5 mg/mL to be SCPN-AF positive, while similar levels of DXT-AF were achieved after 16 hrs with the polymer. After *In vivo* administration, visual inspection of SPECT-CT images suggests that the residence time of SCPN-NODA-Ga nanoparticles and DXT-NODA-Ga polymer is longer than the residence time of control ⁶⁷Ga-Citrate.

Animals sacrifice showed that 40 % of DXT-SCPN-NODA-Ga were cleared from the lung whereas the whole non-crosslinked DXT remained. TEER values of the cell monolayer were measured using MucilAir™ Pulmonary barrier to verify the barrier integrity in presence of DXT-SCPNs. It was found that TEER remained constant after exposure to DXT-SCPNs and therefore this system is not expected to alter the pulmonary epithelium.

Conclusions

Herein, we provide evidence of the better internalization of SCPNs by lung cells compared to the corresponding non-crosslinked polymer. The non-crosslinked polymer appeared to accumulate in rat lung whereas DXT-SCPN showed steady clearance, confirming the advantage of using SCPN technology.

Figures

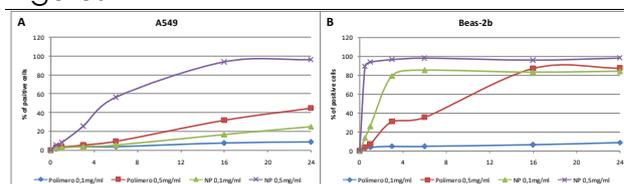


Figure 1. Percentage of SCPN-AF and DXT-AF positive cells after 24 hours of SCPN-AF incubation.

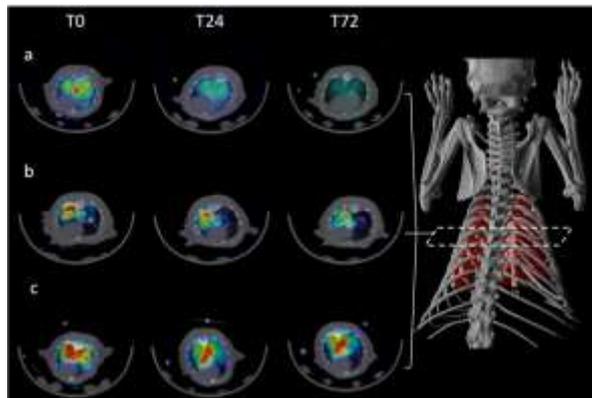


Figure 2. Left: SPECT-CT images obtained at 0, 24 and 72 hours after intratracheal nebulization of ⁶⁷Ga-Citrate (a), DXT-NODA-Ga (b), SCPN-NODA-Ga (c). Right: 3D-rendered CT image of the skeleton (grey tones) coregistered with a 3D-rendered image of the lungs (in red).

Fine-tuning of the nanoporous alumina photonic stopbands by using non-conventional pulse anodization

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Photonic stopbands structures (PSB) based on nanoporous anodic alumina (NAA) are engineered by different periodic anodization of aluminum under specific conditions. The optical properties of NAA structures rely intrinsically upon its nanoporous architecture, and on the geometry and distribution of its nanopores, which can be precisely engineered during the anodization process [1, 2, 3]. Some intrinsic properties such as photoluminescence can also be modified during and after their anodization.

Here we present a novel pulse anodization approach using a gaussian current density profile to engineer NAA photonic crystals with tuneable photonic bands in the UV-Vis-NIR spectral range.

The relationship between the technological parameters and the characteristic features of the photonic stopbands were successfully assessed.

The results provide insights onto optimal anodization conditions to fabricate high-quality NAA-based photonic crystals, opening new opportunities to engineer high-quality structures for light-based technologies such optical sensing, photocatalysts for green energy generation and environmental remediation, optical encoding and lasing [4, 5, 6].

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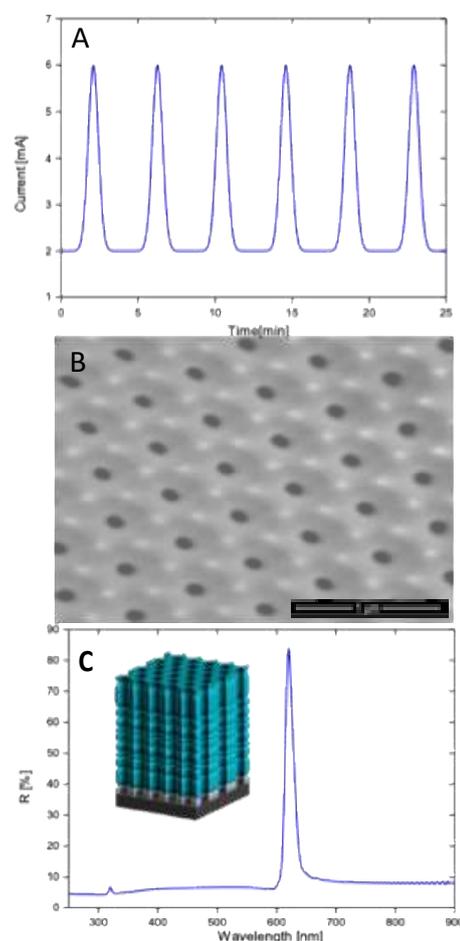


Figure 1: **A.** Gaussian pulse anodization current density profile. **B.** Top view ESEM image of NAA. **C.** Reflection spectrum of a gaussian NAA photonic crystal. Inset a schematic cross-section of the photonic structure.

Graphene-based biosensors

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Abstract

Graphene oxide (GO) and graphene quantum dots (GQDs) display advantageous characteristics with interest for building innovative biosensing platforms and even smart devices such as nano/micromotors for a myriad of uses including sensing. Quenching of the fluorescence induced by GO or photoluminescence of GQDs can easily operate in synergy with various other nanomaterials and platforms opening the way to several unprecedented biosensing strategies and unique nanomotor technologies. Taking advantage of GO, GQDs we are developing simple, sensitive, selective and rapid biosensing platforms that include: a) GO – based microarray & laterals flow technologies taking advantages of high quenching efficiency of GO. A “turn ON by a pathogen” device will be shown as a highly sensitive detection system using plastics or paper/nanopaper substrates; b) GQDs–based sensors for contaminants detection based on the use of multifunctional composite materials that enable rapid, simple and sensitive platforms in connection to smartphone; c) A water activated GO transfer technology using wax printed membranes for fast patterning of a touch sensitive device with interest for electronic devices including sensing as well as for a cost-efficient nanomotor building technology for several applications. This work is supported by EU (Graphene Flagship), CERCA Programme / Generalitat de Catalunya.

Biofabrication to control cell fate

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Organs are complex systems, comprised of different tissues, proteins, and cells, which communicate to orchestrate a myriad of functions in our bodies. Technologies are needed to replicate these structures towards the development of new therapies for tissue and organ repair, as well as for in vitro 3D models to better understand the morphogenetic biological processes that drive organogenesis. To construct tissues and organs, biofabrication strategies are being developed to impart spatiotemporal control over cell-cell and cell-extracellular matrix communication, often through control over cell and material deposition and placement. Here, we present some of our most recent advancements in biofabrication that enabled the control of cell activity, moving towards enhanced tissue regeneration as well as the possibility to create more complex 3D in vitro models to study biological processes.

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Figures

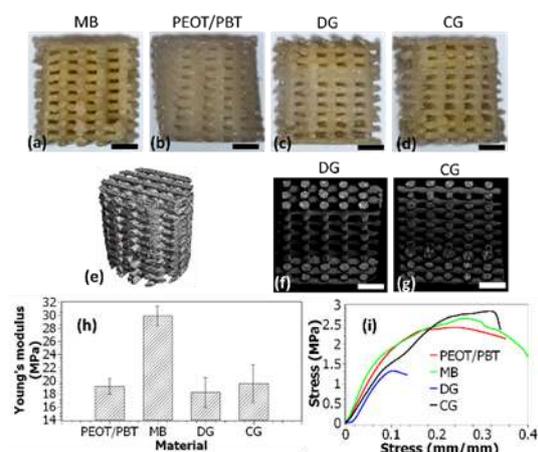


Figure 1: Representative scaffold images: stereomicroscope (a-d), μ CT (e), BSE-SEM (f-g); calculated moduli (h), and stress-strain curves (i).

Shaping light using ultrafast and programmable nano-optics

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Abstract

A variety of applications requires light and infrared radiation to be shaped and controlled actively. In our laboratory we are working on shaping light using silicon photonics on a chip [1] and in free space using metasurfaces [2]. Key to these applications are materials that can be tuned or switched optically, electrically or thermally. In this presentation I will give an overview of cutting edge developments in shaping of light using phase change materials [2,3] and ultrafast all-optical perturbations [1]. I will also address efforts at modelling these effects using emerging new techniques from the toolbox of machine learning [4].

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Figures

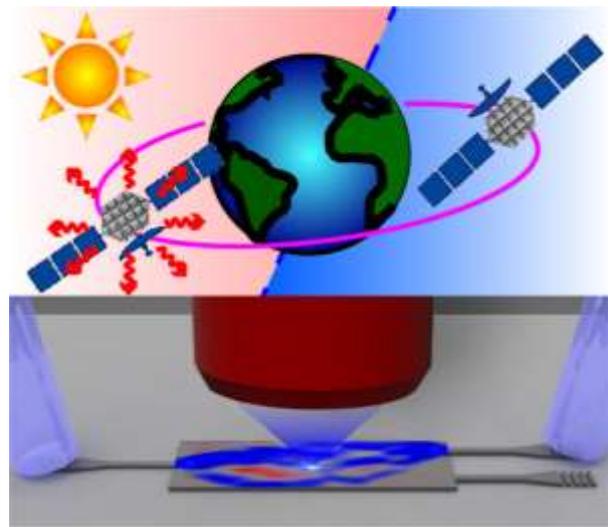


Figure 1: Examples of applications of control of infrared radiation (top, smart solar reflector using VO₂ metasurface) [2] and on-chip programmable photonics (bottom) [1].

Graphene based Electronic Devices and Integrated Circuits – Applications and Manufacturing

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Radio frequency integrated circuits (RF ICs) built the core of modern information and communication systems. Graphene based devices like transistors, diodes or varactors have been recognized from the very beginning as promising candidates in future RF ICs, having the potential to significantly outperform established devices based on Silicon or III/V semiconductor materials in terms of speed, functionality or mechanical flexibility.

However, so far the potential of graphene in RF electronics has mainly been demonstrated on a single device level because the realization of more complex integrated RF circuits was limited by a non-mature fabrication technology and large variations in the device performances.

In this presentation I will first present the MMIC (monolithic microwave integrated circuit) process for graphene based RF circuits developed at AMO and discuss especially the challenges and possible solutions related to device variability and yield.

Different RF ICs have been realized so far, which are designed for future WiFi communication systems in 5G and for IoT applications.

In the second part of the presentation, I will discuss approaches, challenges and possible solutions for the wafer scale integration of graphene based electronic and sensor devices [1]. The performance will be compared to chip scale production and the current limitations for yield, device to device variation and reproducibility will be discussed.

References

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Figures

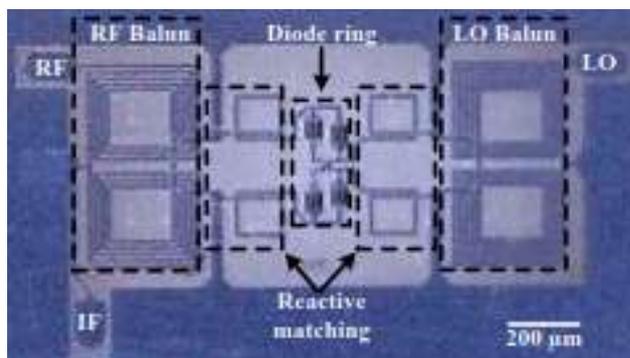


Figure 1: Optical micrograph of an integrated RF circuit (double balanced mixer operating at 6-12 GHz). The different parts of the circuit are indicated.

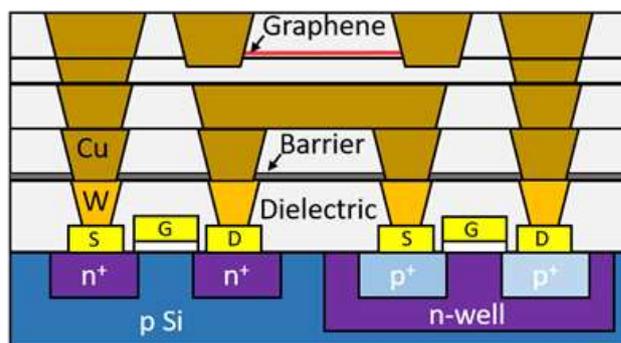


Figure 2: Possible integration scheme of graphene into a silicon CMOS platform at the back-end-of-the-line, as it could be used for graphene based Hall Sensors.

Discovery of the intrinsic antiferromagnetic topological insulators: theory and experiment

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Using *ab initio* methods, we predict the van der Waals layered compound MnBi_2Te_4 (MBT) to be the first antiferromagnetic topological insulator (AFMTI) [1-3]. The interlayer AFM ordering makes MBT invariant with respect to the combination of the time-reversal (θ) and primitive-lattice translation ($T_{1/2}$) symmetries, $S=\theta T_{1/2}$, which gives rise to the Z_2 classification of AFM insulators, $Z_2 = 1$ for this material. The S -breaking (0001) surface of MBT exhibits a band gap in the topological surface state thus representing an ideal platform for the observation of the quantized magnetoelectric coupling and intrinsic axion insulator state. Our prediction is confirmed experimentally by means of structural, magnetic, and photoemission spectroscopy measurements [1]. In the 2D limit, MBT is expected to show a unique set of thickness-dependent magnetic and topological transitions, which drive it through FM and (un)compensated AFM phases, as well as quantum anomalous Hall (QAH) and zero plateau QAH states [4]. Thus, MBT is the first stoichiometric material predicted to realize the zero plateau QAH state intrinsically. This state was earlier predicted to host the axion insulator phase. The discovery of the first AFMTI opens a new field of magnetic TIs that focuses on intrinsically magnetic stoichiometric compounds [5-8]. Finally, apart from MBT itself, its FM building blocks can be used for creation of topological heterostructures [9-12].

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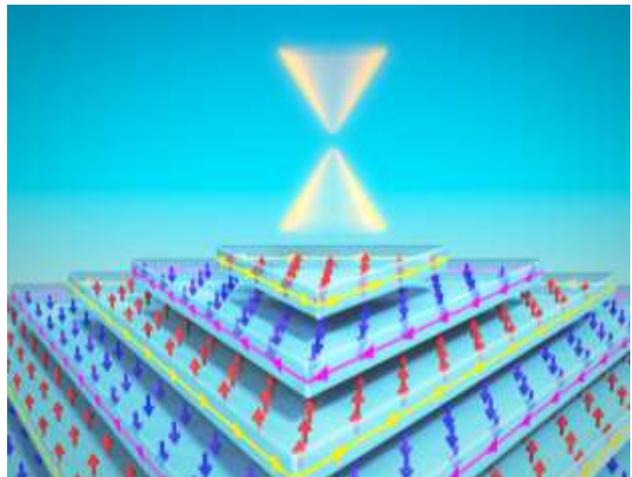


Figure: Artistic representation of the stepped surface of MnBi_2Te_4 , and above, the characteristic electronic feature of an AFMTI, the so-called Dirac cone. The red and blue arrows represent the local magnetic moments of the Mn atoms, whose directions alternate from one terrace to the next (antiferromagnetic order). The yellow and pink lines and their respective arrows show the directions of

propagation of the electric currents at the borders, which are opposite between neighbouring borders, which is known as Half-integer quantum Hall effect.

Single-Chain Nanotechnology: Current Status and Opportunities

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The recent ability to manipulate and visualize single atoms at atomic level has given rise to modern bottom-up nanotechnology. Similar exquisite degree of control at the individual polymeric chain level for producing functional soft nanoentities is expected to become a reality in the next few years through the full development of so-called “single chain nanotechnology”. Ultra-small unimolecular soft nano-objects endowed with useful, autonomous and smart functions are the expected, long-term valuable output of single-chain nanotechnology.

This keynote lecture focus on the recent advances in single-chain nanotechnology for the construction of soft nano-objects via chain compaction, with special emphasis in single-chain nanoparticles (SCNPs). [1] SCNP formation is reminiscent of protein folding and depending on the synthesis route and the amphiphilic nature of the SCNP precursor two limiting SCNP molecular architectures result: *Type I*-SCNPs with multiple “local pockets”, and *Type II*-SCNPs with a single pocket of larger size. The possibility to anchor, either temporally or permanently, active species like drugs or catalysts onto these local pockets paves the way to the use of SCNPs in a variety of nanomedicine and catalysis applications.

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Figures

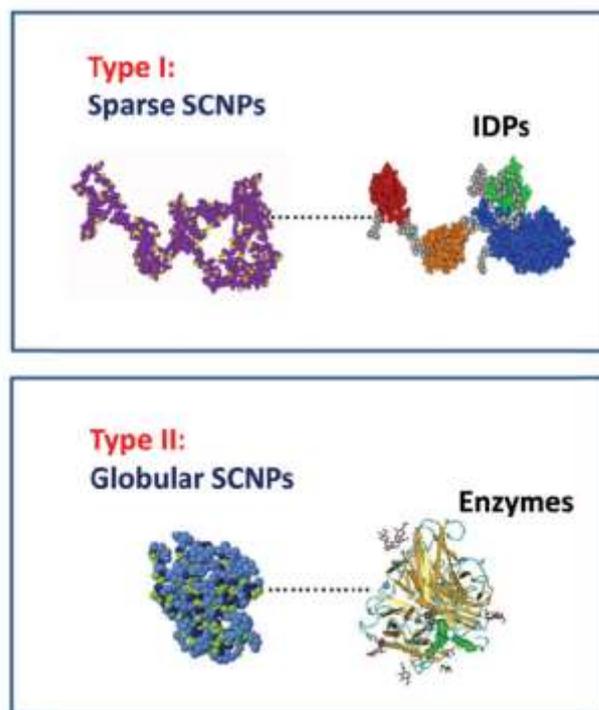


Figure 1: Morphologies of single-chain nanoparticles (SCNPs).

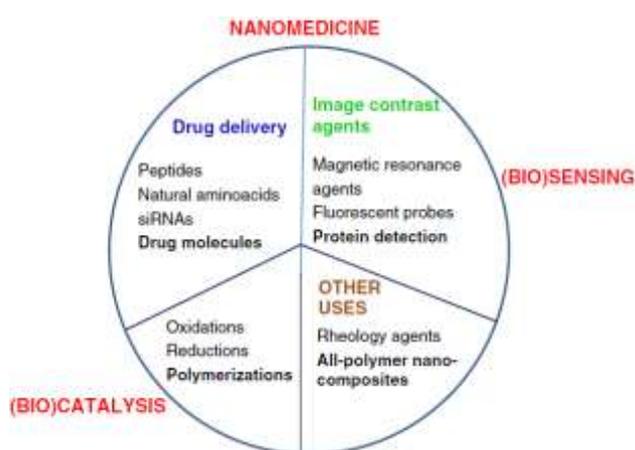


Figure 2: Application areas for SCNPs.

Integration of Microphysiological Systems with Organ-on-a-Chip technology for Disease Modeling

Javier Ramón-Azcón^{1,2}

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The pharmaceutical industry relies heavily on in vivo animal models and in vitro 2D cell cultures to develop therapeutic strategies. There are many ethical issues surrounding animal studies and serious concerns also exist regarding their biological relevance to humans. Particularly, current 2D tissue models often do not simulate complex cell-cell and cell-matrix interactions, which are crucial for regulating cell behaviours in vivo. Due to these shortcomings, there is now substantial interest in developing fully functional 3D tissues that mimic the in vivo system closely as possible for the disease modelling and chemical testing. Recent advances in miniaturizing microfluidic systems and advanced tissue fabrication procedures have enabled researchers to create multiple organs-on-a-chip with a high degree of control over experimental variables for high-content screening applications. However, there is a gap in the integration of these potential platforms to sensing modules, capable to monitor in real-time fast metabolic behaviours subjected to external stimuli, like stress or drugs.

In our work, three 3D engineered tissues (liver, pancreas and skeletal muscle)¹⁻⁴ are integrated with new real-time sensing technology on a single platform to obtain a reliable model to study diabetes type II disease and related metabolism, detecting and monitoring real-time cellular responses to external stimuli. Bringing this together coherently will deliver the prize of a deep understanding of the metabolic system with applications spanning drug development, diabetes related medical devices and increased prognosis of metabolic system related conditions.

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FIGURES

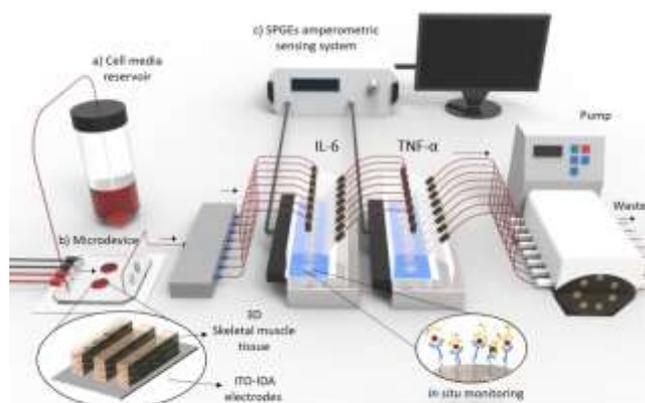


Figure 1: Schematic overview of the configuration and function of the muscle-on-a-chip⁴.

Near-field Interference for Local Field Shaping

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Abstract:

Optical nanoantennas are well-known for the confinement of light into nanoscale hot-spots, suitable for emission enhancement and sensing applications. Here, we show how control of the antenna dimensions allows tuning the local optical phase, hence turning a hot-spot into a cold-spot [1]. We manipulate the local intensity exploiting the interference between driving and scattered field. Using single molecules as local detectors, we experimentally show the creation of subwavelength pockets with full suppression of the driving field. Exploiting the local interference we demonstrate position control of the localised field i.e. the plasmonic hotspots in the near-field of a nanoantenna [2]. Remarkably, together with the cold excitation spots we observe inhibition of emission by the phase-tuned nanoantenna. The fluorescence lifetime of a molecule scanned in such volumes becomes longer, showing slow-down of spontaneous decay. In conclusion, the spatial phase of a nanoantenna is a powerful knob to tune between enhancement and inhibition in a 3-dimensional subwavelength volume. Moreover, the interference effect can be exploited to shape the nanoantenna near-field to produce a tailored optical response such as polarization-controlled nanoscale hotspot switching, as we show here [1-3].

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FIGURES

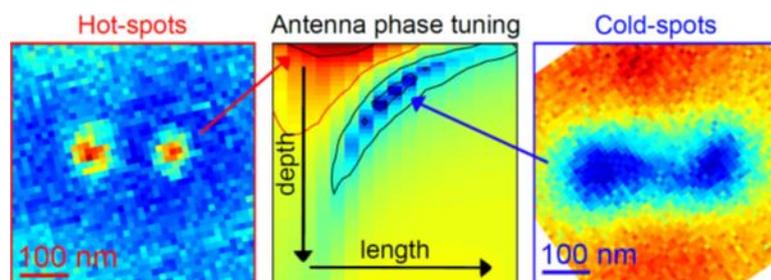


Figure 1:

Hot and Cold Spots: from Enhancement to Suppression by Nanoscale Phase Tuning of Optical Nanoantennas

● INVITED

Graphene devices for biosensing applications

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Abstract

The importance of biosensors in biomedical research keeps increasing at a fast pace, as they are routinely used in a wider range of applications. Graphene low-dimensionality, as well as its high carrier mobility and chemical stability, allows to fabricate relatively simple, label free, highly sensitive biosensors, based on different types of devices [1]. Here, we propose the development of a miniaturized biosensing platform based on liquid-gate graphene field-effect transistors (GFETs) achieving detection of DNA hybridization down to attomolar concentration, while being able to discriminate a single nucleotide polymorphism (SNP) [2].

In another approach, we use the z^{-4} nanoscale distance-dependence of the fluorescence lifetime for fluorophores located in the vicinity of graphene to track the hybridization of fluorescently labelled DNA beacons attached to CVD grown graphene with complementary (target) DNA added in solution. We follow the conformational changes of the beacons by determining the fluorescence lifetimes of the labelling dye and converting them into nanoscale distances from the graphene. In this way, we are able to monitor the vertical displacement of the label during DNA-beacon hybridization with an axial resolution reaching down to 1 nm [3].

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Figures

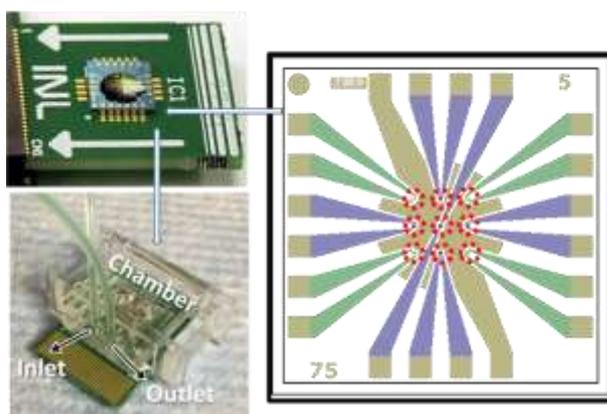


Figure 1: (counterclockwise from right to left) The sensor chip containing 9 GFETs (highlighted in red) is wire-bonded to a PCB to be inserted in the control board. A PDMS flow cell, fitting the sensor layout, can be assembled to the chip prior to insertion in the board.

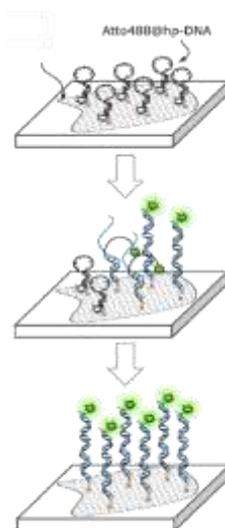


Figure 2: Initially, before the hybridization with target DNA the beacons are in the folded configuration. Upon DNA hybridization, the labeling dye is displaced away from the graphene, and its fluorescence is restored in dependence of the nanoscale distance to graphene.

Mechanically stable graphene with quadratic out-of-plane acoustic modes

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The phonon properties of 2D materials are far from trivial as the harmonic approximation predicts fast diverging atomic displacements as a function of the sample size and finite linewidths of the longitudinal and transverse in-plane acoustic phonon modes at small momenta. These problems arise due to the quadratic dispersion of the acoustic out-of-plane phonon frequencies obtained in the harmonic approximation. By including anharmonicity within the self-consistent harmonic approximation (SCHA) we show that the divergences in the atomic displacements are suppressed and the linewidths of in-plane acoustic phonons vanish at low momenta, recovering the physical picture. By calculating the phonon spectra from the Hessian of the anharmonic free energy, we conclude that the physical dispersion expected experimentally for the acoustic out-of-plane mode should be quadratic (see Figure 1). We verify this result both using atomistic simulations and using a membrane model for graphene. Our conclusions [1] have a crucial role in the understanding of the mechanical and thermal properties of graphene and other strictly two-dimensional material.

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Figures

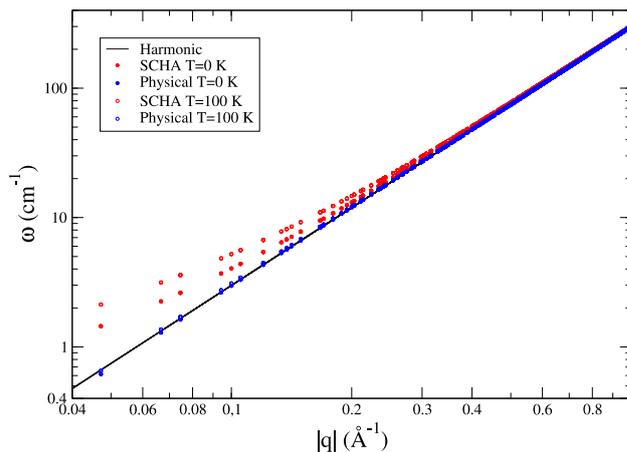


Figure 1: Frequency of the ZA mode in the harmonic approximation, within the SCHA and obtained from the Hessian of the SCHA (labeled as "Physical") both at 0 K and 100K using the membrane model. The physical phonons recover the quadratic dispersion of the harmonic solution.

Graphene based composites becomes a reality in 2020

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Abstract (Century Gothic 11)

The application bulk graphene materials in composites is predicted to be the largest market for graphene, followed by energy storage [1]. Several reviews analysed the applications of the different graphene and related products in composites. [2, 1b] Several products based on composites, mainly in sport good sector, claims that are based on graphene materials. Sport good sector only represent less than 3 % of the whole composite market.[3]

In this presentation we will report the potential market and actual large volume application in the polymer composites sector.

Several new applications and the use of GRMs in products will be reported.

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Figures



Figure 1: GRM application in rubber



Figure 2: Application of GRMs in a thermoplastic

Magnetic hyperthermia for cancer treatment: past problems, ongoing work and future possibilities

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Magnetic nanoparticles (MNPs) emerged more than two decades ago as promising tools for several biomedical applications such as contrast agents, drug delivery systems or heat mediators in magnetic hyperthermia. Recently, new approaches for cancer treatment based on the production on heat that go one step further than traditional hyperthermia have been developed. Instead of focusing just on the heat generation to induce cell death, the main aim of these new approaches is to use the temperature increase as a stimulus to trigger different reactions or transformations in the surrounding environment.

In this talk, first, a critical review of the research performed in the past decades on magnetic hyperthermia will be presented. Then, current work related to the use of magnetic hyperthermia as a tool to increase the permeability of the extracellular matrix in tumour models will be discussed. The analysis of 3D cell cultures [1] and tumour tissues will be shown paying special attention to problems observed to achieve a satisfactory treatment. Finally, aspects to considered to improve the effectiveness of the treatment will be indicated.

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Figure

Increase of the extracellular matrix permeability after magnetic hyperthermia

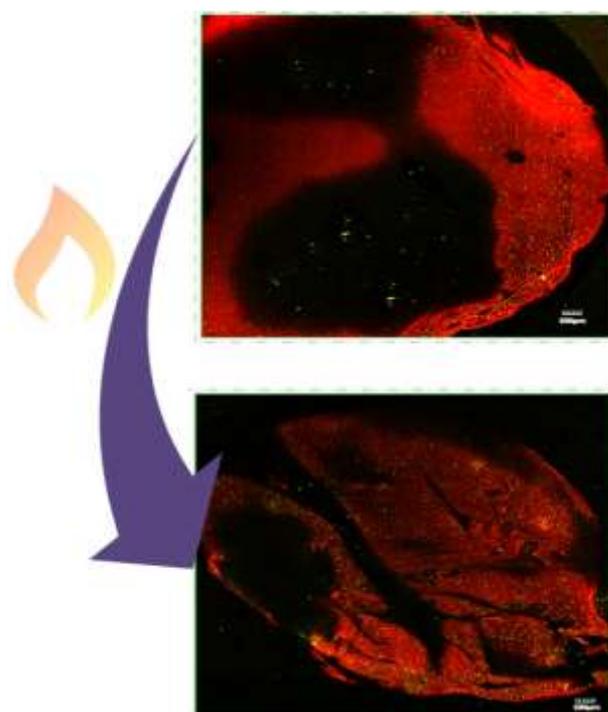


Figure 1: Map image of confocal microscopy of 3D cell culture without (up) and with (down) the alternating magnetic field exposure. The image shows the overlay of two channels: green fluorescence of the labeled cells and red fluorescence of the magnetic nanoparticles. Scale bar is 500 μm .

Magneto-optical Stern-Gerlach forces and non-reciprocal torques on small particles

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Abstract

In this work, we calculate the optical forces [1] and torques caused by the presence of a sizeable magneto-optical effect [2]. We find a conservative force proportional to the gradient of the spin density of the light field and an extinction force proportional to the helicity of the light field. The conservative interaction allows for a spin-selective, magnetic field based Stern-Gerlach experiment, capable of differentiating between right and left circular polarizations (see Figure 1). We also prove that by using a spin-less linearly polarized plane wave, the magneto-optical effect allows for the existence of a permanent non-reciprocal torque, proportional to the intensity of the light field [3].

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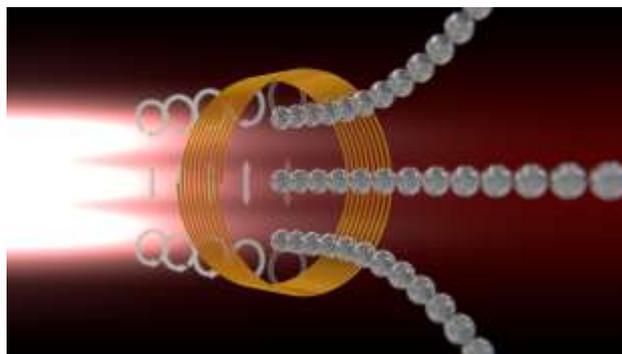


Figure 1: Spin-selective, magnetic field based Stern-Gerlach experiment, capable of differentiating between right and left circular polarizations

Figure 2: Insert caption to place caption below figure (Arial 10)

Bioengineering enzyme-powered nanomachines for nanomedicine: from *in vitro* studies to *in vivo* imaging

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Abstract

Inspired by nature, researchers have been exploring the rich multifunctionality of molecular motors, cells and other microorganisms to engineer artificial smart nanosystems able to move, interact with their environment and perform complex tasks at the nanoscale. Recently, artificial nanomachines that harness chemical energy from *in situ* chemical reactions and convert it into active motion have been developed. Particularly, enzymes are powerful biological catalysts that convert substrates into products.[1] By harvesting this chemical energy, enzymatic micro- and nanomachines are able to self-propel. These motor-fuel complexes hold a great potential towards nanomedicine thanks to their versatility, bioavailability and full biocompatibility. Although the field is still in its infancy, several milestones have been reached, such as enhanced anti-cancer drug delivery [2] specific targeting and penetration in 3D bladder cancer spheroids. [3] However, when biomedical applications are envisaged, several fundamental questions need to be resolved: what are the optimal design features of enzyme-powered nanomachines? How do they behave in physiologically relevant media? How can we monitor their actuation *in vivo*? In this talk, I will present our last developments on enzyme-powered nanomachines, from understanding the fundamental aspects behind their self-propulsion[4] to *in vitro* drug delivery systems,[5] sensing,[6] and *in vivo* real time monitoring.[7]

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Graphene Oxide for Functional Coatings

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Abstract

Graphene oxide being a two-dimensional material with a high density of functional groups is an obvious candidate material for functional coatings of different kinds. Abalonyx is involved in several activities related to functional coatings, internally and in collaboration with partners. Anti-corrosive coatings for auto-parts is already used commercially¹. At our lab, we have recently developed a method for coating of glass-fibers (Fig. 1) with rGO, as an alternative to polymer coating, with the aim to achieve better adhesion between polymer and fibers in glassfiber reinforces polymers. We are also involved in a Manunet project with partners at INOE 2000, SITEX 45, INFLPR, and SINTEF to develop coatings for glass with nonlinear properties showing very promising results. In another project we use electrospaying to deposit thin GO and rGO coatings on a range of substrates. Target applications are protective coatings such as anti-UVA, anti-corrosion and protecting eyes and sensitive optical sensors from laser damage². Another example is rGO-coating on borosilicate depicted in Fig 2 for use in bio-sensing process which offers a fast and label-free approach for analyte detection³.

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Figures



Figure 1: Uncoated and rGO-coated glass-fibers for polymer composite reinforcement.



Figure 2: rGO-coatings on borosilicate glass-slide prepared by electrospaying.

Graphene Commercialisation Status

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Abstract

The properties of graphene make it an ideal candidate to be applied in electronics, photonics, sensors [1-3], energy, etc. Unfortunately, these applications are yet to be materialised since there are many integration challenges that have to be overcome before a new advanced material can be introduced into the market. How this integration will occur will depend on the application and the graphene type (graphene films vs bulk graphene). However, all the integration scenarios will require a scalable, uniform and high-quality graphene. In addition, depending on the application and type of graphene, regulation and toxicity issues could slow down the commercialisation process.

During this talk, I will give an overview of the integration challenges that we face in various graphene applications. Including, how this integration could be accelerated by offering a graphene device fabrication service.

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● ORALS

Infrared permittivity of the biaxial van der Waals semiconductor α -MoO₃ from near- and far-field correlative studies

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The biaxial van der Waals semiconductor α -phase molybdenum trioxide (α -MoO₃) has recently received significant attention due to its ability to support highly anisotropic phonon polaritons (PhPs) —infrared (IR) light coupled to lattice vibrations in polar materials—, offering an unprecedented platform for controlling the flow of energy at the nanoscale, beyond what has been achieved with other materials supporting PhPs. However, to fully exploit the extraordinary IR response of this material, an accurate dielectric function is required. Here [1], we report the accurate IR dielectric function of α -MoO₃ by modelling far-field polarized IR reflectance spectra acquired on a single thick flake of this material. Unique to our work, the far-field model is refined by contrasting the experimental dispersion and damping of PhPs, revealed by polariton interferometry using scattering-type scanning near-field optical microscopy (*s*-SNOM) on thin flakes of α -MoO₃, with analytical and transfer-matrix calculations, as well as full-wave simulations. Through these correlative efforts, exceptional quantitative agreement is attained to both far- and near-field properties for multiple flakes, thereby strongly verifying the accuracy and robustness of our model, while offering a novel approach to extracting dielectric functions of nanomaterials, usually too small or inhomogeneous for establishing accurate

models only from standard far-field methods. In addition, by employing density functional theory (DFT), we provide insights into the various vibrational states dictating our dielectric function model and the intriguing optical properties of α -MoO₃.

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Figures

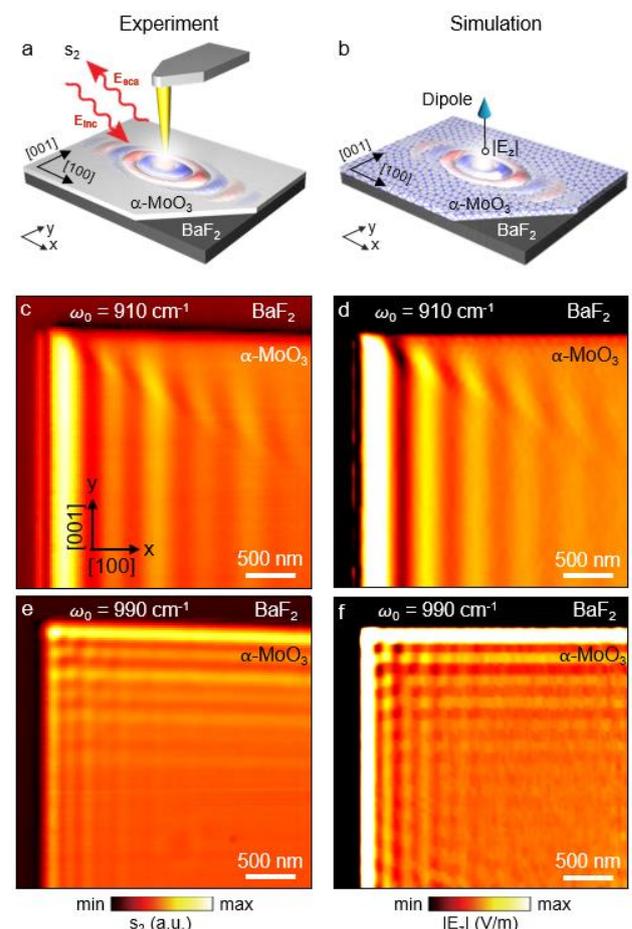


Figure 1: Near-field simulated and experimental images of in-plane anisotropic PhPs on an α -MoO₃ thin flake.

On-Surface Boroxine 2D Covalent Organic Frameworks: a Comprehensive Analysis

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Gaolei Zhan,^a Cristina Martín,^b Kunal S. Mali,^a Aurelio Mateo-Alonso,^c Mark Van der Auweraer,^a Steven De Feyter^a

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Two-dimensional covalent organic frameworks (2D COFs) are a type of porous, organic and crystalline 2D material.^[1] Although they display very interesting properties, the industrial application of 2D COFs is still limited by the poor control over their synthetic and interfacing processes. Here, we describe a simple protocol to prepare large and defect-free single-layer 2D COFs under mild conditions, at room temperature and at the liquid-graphite interface. Using scanning probe microscopy (SPM) and a variety of spectroscopy techniques, we reveal at the molecular level the impact of monomer concentration, solvent, temperature, and time, bringing mechanistic insight to on-surface COF formation (Figure 1).^[2]

Acknowledgements.

Funding from the Fund of Scientific Research-Flanders (FWO) is gratefully acknowledged.

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Submitted.

Figures

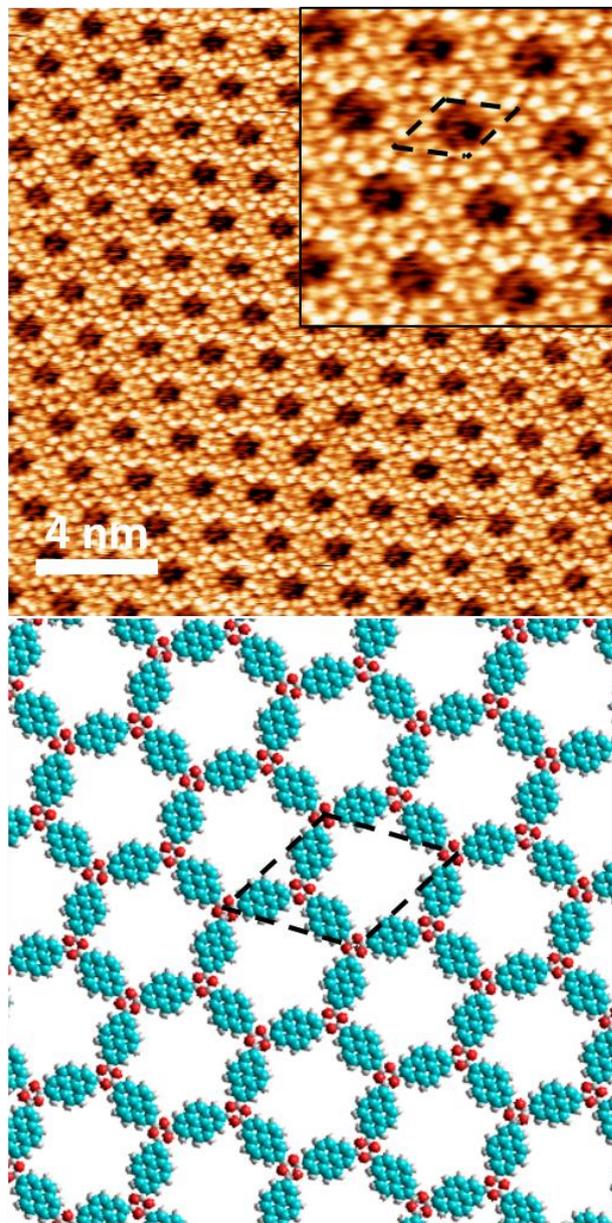


Figure 1: High-resolution STM image of a boroxine COF on graphite and corresponding molecular model.

Synthesis, Characterization and Properties of Silver Clusters

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Subnanometric metallic clusters are getting considerable attention recently due to their properties, which are very different from the bulk or nanoparticle ones, offering exciting possibilities for their use in novel materials or devices, in different fields like medicine, magnetism or catalysis [1]. A subnanometric cluster is a metallic molecule having between 2 and ≈ 20 atoms with a fixed geometry and, due to its reduced size, a well-defined bandgap at the Fermi level (larger as smaller is the cluster), which grants them new electronic structure that determine the appearance of completely new properties strictly depending on the size of the cluster. In fact, changes in one or two atoms, will affect the bandgap thus changing completely their properties [2,3, 4]. Therefore, the design of efficient synthetic methods for the size-controlled synthesis of monodisperse samples of clusters is required. Here, we report the electrochemical synthesis of fluorescent Ag clusters in water without any surfactant or protecting agent by using the so-called kinetic control techniques [4]. The main factors affecting the stability and cluster size will be addressed. Clusters were characterized by UV-Vis spectroscopy, Fluorescence Spectroscopy and Mass Spectrometry. The developed synthesis opens up different possibilities for their application in different fields (due to the small bandgap and the low energy position of the HOMO) like visible photocatalysis.

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FIGURES

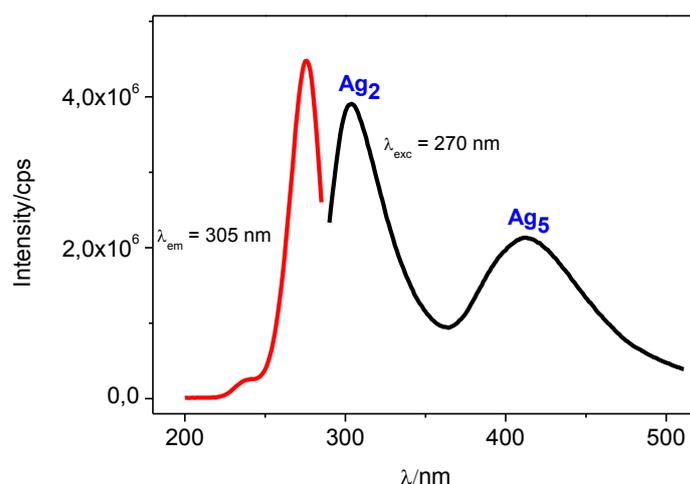


Figure 1: Photoluminescence characterization of a sample of Ag nanoclusters mostly composed by Ag₂ and Ag₅ clusters. Excitation (red line) and emission (black line) spectra.

TUNING TITANIUM DIOXIDE WITH Cu_5 -ATOMIC QUANTUM CLUSTERS FOR HYDROGEN PHOTOPRODUCTION

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Atomic quantum clusters (AQC) are particles formed by small number of atoms of a metal (less than ≈ 100). They present novel properties such as fluorescence, catalysis, photocatalysis, and biomedical properties that differ from both nanoparticles and bulk of the same material. These properties depend strictly on the cluster size.[1] AQC are not metallic, they are semiconductors whose band gap energy is tunable by the size. The smallest AQC the biggest bandgap, becoming really promising in photocatalytic applications.

TiO_2 is a popular semiconductor used in photocatalytic applications, but its main limitation is the lack of light absorption on the visible. The optical response of TiO_2 changes in presence of Cu_5 -AQC increasing and moving the absorption from ultraviolet region to visible. The optical response is measured by diffuse reflectance spectrometry (DRS) (Figure 1A). The Cu_5 interact with TiO_2 transferring an electron and creating a polaron (Ti^{3+}) that is characterized by electron-paramagnetic resonance (Figure 1B).

The hydrogen photoproduction reaction is carried out in the presence of a hole scavenger, triethylamine. TiO_2 doped with Cu_5 increases its hydrogen production due to increased absorption in the visible region and the appearance of the surface polaron with a theoretical bandgap of 0.9 eV [2, 3]. One of the principal problems in photocatalysis is the pair electron-hole recombination that is avoided too by polaron appearance that induces the charges separation.

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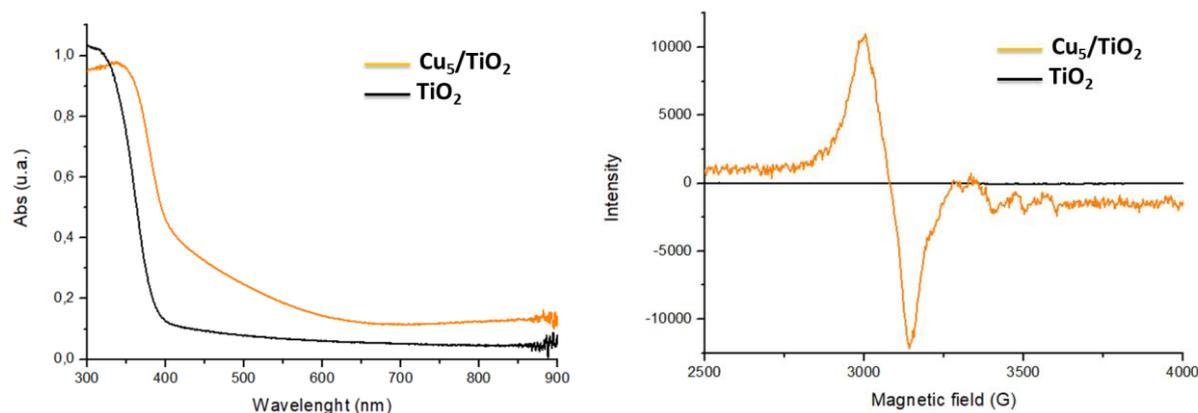


Figure 1: (A) UV-vis absorption spectra of TiO_2 undoped and TiO_2 doped with Cu_5 -AQC. (B) EPR spectra of TiO_2 undoped and TiO_2 doped with Cu_5 -AQC.

A nanotechnological entry to fine carbohydrate-protein detection through CVD graphene

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Mass spectrometry (MS) is a valuable tool for functional genomics, proteomics, and glycomics studies. In particular, the combination of MS with microarrays is a powerful technique for analyzing the activity of carbohydrate processing enzymes and for the identification of carbohydrate-binding proteins (lectins) in complex matrices. On the other hand, graphene exhibits high desorption/ionization efficiency, good conductivity and optical transparency, specifications of a high-performance component for laser desorption/ionization (LDI) platforms.[1] However, current substrates are far from ideal in terms of stability, reproducibility and effective functionalization; thus, improved performance with new materials is demanded.

In this work, the potential of Chemical Vapour deposited graphene (CVDG) as a performance component for LDI-MS analysis is reported for the first time. In particular, the use of CVDG as a platform for the preparation of glycan arrays to monitor carbohydrate-lectin interactions by MS and fluorescence is described. In this array, CVDG behaves as anchoring platform, as conductive material and as matrix-free LDI surface. Likewise, the crucial role of

chemical functionalization for the manufacture of CVDG carbohydrate microarrays is discussed.

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Figures



Figure 1: General representation of preparation of CVDG-based carbohydrate microarrays for dual mass spectrometry and optical microscopy readout. As example, Lewis^x carbohydrate structure is represented.

Plasmonic supercrystals integrated in microfluidics for ultrasensitive and selective SERS detection

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Surface-enhanced Raman spectroscopy, SERS, is an advanced analytical technique that can be used for the ultrasensitive detection of analytes. It is based in the enhancement of the Raman signal of a molecule at the surface of a plasmonic nanostructure mainly due to the presence of strong electromagnetic fields generated after the plasmon excitation. Moreover, this effect could be more intense in the case of plasmonic supercrystals due to antenna effects as demonstrated by recent simulations.¹

As we previously reported, microfluidic platforms allow generating a highly-ordered assembly of uniform gold nanoparticles inside their microchannels through the slow pervaporation of the solvent (Figure 1A-B).² While plasmonic supercrystals made by drop-casting show poor uniformity that limits their potential plasmonic applications.³ Microfluidic approach enables the fabrication of supercrystals of any dimension or morphology. Furthermore, the integration of a plasmonic supercrystal inside microfluidic platform guarantees the infiltration of the desired analyte, even without affinity for gold surface, within the plasmonic supercrystals and therefore its ultrasensitive detection.

Herein, we show the fabrication and characterization of plasmonic supercrystals using gold octahedra nanoparticles synthesized through a wet chemical method. Besides, the study of the sensing capabilities of these platforms showed a highly uniform and intense SERS activity (Figure 1C), being both key parameters to achieve quantitative and ultrasensitive analysis (LOD) (Figure 1E).⁴ In fact, LOD as low as 10^{-19} M was achieved for the detection of Crystal Violet (CV), which is several orders of magnitude lower than those found in the literature. Also, we investigate the possibility of combining the capabilities of our SERS sensor with the chromatographic properties of silica nanoparticles to develop a sensor device with the ability of separate analytes by charge (Figure 1D).

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FIGURES

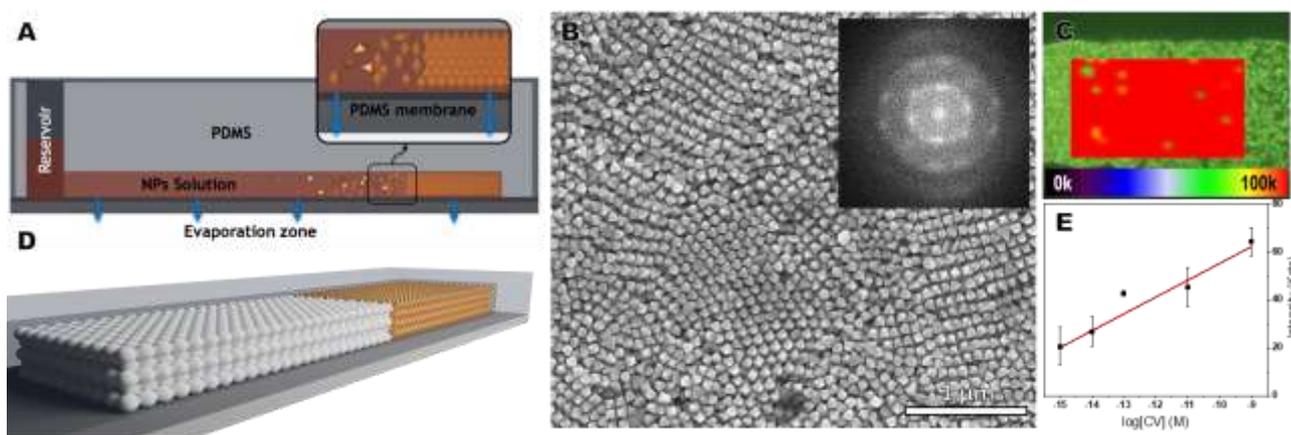


Figure 1: (A) Schematic illustration of self-assembly of gold octahedra nanoparticles inside microfluidic platform induced by pervaporation. (B) Scanning Electron Microscopy (SEM) image of the supercrystal. Inset corresponds with the result of applied Fourier Transform (C) SERS hot-map obtained at 1617 cm^{-1} in the presence of 10^{-7} M of CV. (D) Schematic representation of the final SERS Sensor modified with a silica supercrystal for chromatographic separation. (E) SERS intensity obtained for different concentrations of CV (10^{-7} - 10^{-14} M).

Photoluminescent Organic Materials with Tuneable Emission-Colour and Polarization

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The controlled organization of π -conjugated systems at the molecular, nano- and microscales can lead to materials with exceptional optoelectronic properties. Self-assembly pathways can be controlled by molecular design, concentration, additives, solvent conditions, and temperature [1]. Their optical properties result from tailored molecular design, molecular packing, shape and size, incorporation of suitable dopant-molecules and excitation dynamics [2].

Figures

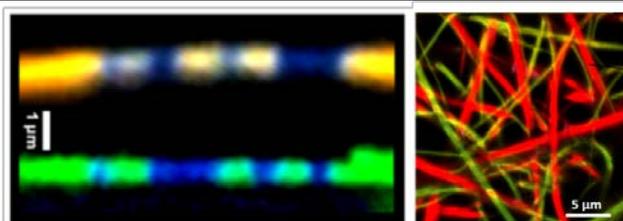


Figure 1: Left: Hyper-spectral map of an orange and a green ribbon patterned in presence of ambient oxygen. Right: Hyper-spectral map of an interpenetrated orthogonal ribbon network.

FRET-amplified photo-patterning is proposed as a new strategy for sub-micrometer scale colour-tuning in self-assembled fluorescent nano-ribbons formed by n-acenes [2]. This allows individual ribbons to be colour-tuned locally at a microscopic level (Figure 1, left) with high linear emission polarization. Thereby, combining different molecules

and photochemistry at the sub-micrometer scale under the microscope, colourful patterned ribbons could be obtained.

In addition, orthogonal assembly was exploited to grow interpenetrated networks of two novel n-acene derivatives. This study presents a first example of efficient separation between analogue structures, by controlling the self-assembly pathways. These two alkoxyated fluorophores assemble into two separated interpenetrated fiber networks, yielding two-colour emission from the orthogonal gel (Figure 1, right). Interesting changes in optical properties are observed by altering the solvent composition, realizing different colours in consequence of differing molecular packings and thus dipolar coupling. At the hetero-crossings inter-object energy transfer and electroluminescence can be observed.

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Funding: EC Marie Curie ITN project SMARTNET and Basque Government Postdoctoral Fellowship (L.G-R).

Optomechanical detection of single bacterium mechanical modes

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

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Figures

Figure 1: Frequency of the radial breathing mode of a 320 nm thick optomechanical disk (blue region) and of the fundamental mode of a quasi-spherical biological particle adsorbed on a rigid support (red region), as a function of the disk and bioparticle radii, respectively.

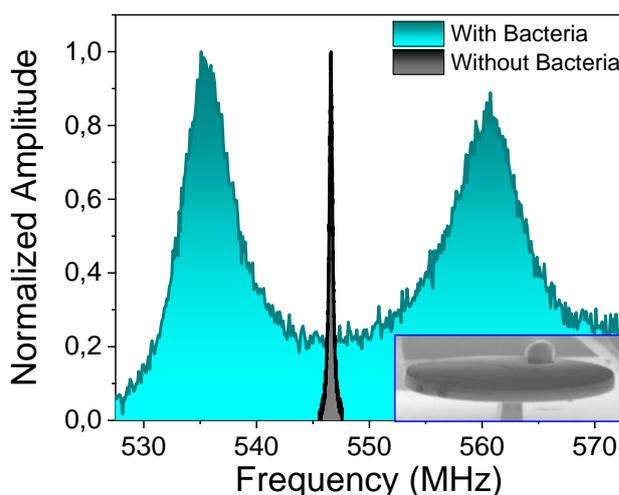


Figure 2: Effect of bacterium adsorption on the radial breathing mode of an optomechanical disk (2.5 μm in radius and 320 nm in thickness). The inset shows a scanning electron microscopy image of the optomechanical disk with an attached *Staphylococcus epidermidis* cell.

NanoFrazor lithography for precise shaping and non-invasive contacting of 1D & 2D materials

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Thermal scanning probe (t-SPL), or NanoFrazor lithography is the first true alternative to electron beam lithography (EBL), with the tools readily available on the market [1]. A heatable NanoFrazor tip patterns by locally evaporating resist materials and inspects the sample as an atomic force microscope (AFM). The heated tip can pattern very high-resolution nanostructures (<10 nm half-pitch). The cold tip inspects nanostructures before, during and after the patterning process, enabling stitching and markerless overlay with sub-5 nm accuracy [2]. t-SPL is compatible with all common pattern transfer processes [3,4,5]. It is particularly suitable for shaping 2D materials into narrow ribbons or Hall bars and for making high-quality electrical contacts on them. Here, we show that NanoFrazor lithography can yield high-quality metal electrodes or top gates [3,5], Figures 1 and 2, and shape 2D materials with very high precision [6]. The resulting devices exhibit vanishing Schottky barrier height (~ 0 meV), record-high on/off ratios of 10^{10} , no hysteresis, and subthreshold swing (SS) as low as 64 mV per decade [5].

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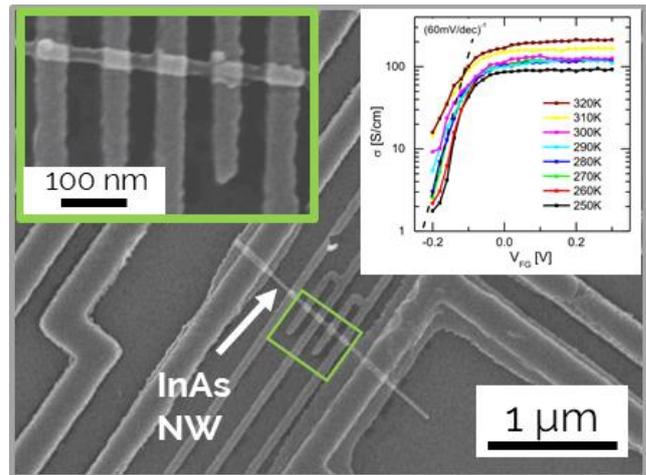


Figure 1: SEM image of an InAs nanowire FET with top gates fabricated using t-SPL. Direct sublimating of the resist prevents charge accumulation in the Al_2O_3 gate dielectric; Left inset: a close-up marked by the green frame; Right inset: the device's performance at different temperatures and $\text{SS} = 60$ mV per decade. [3]

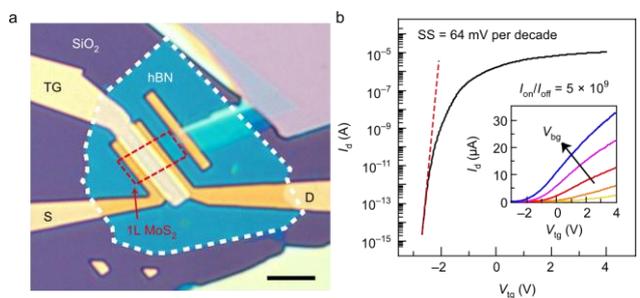


Figure 2: a) 1L-MoS₂ double-gated field-effect transistor (FET) with h-BN as a gate dielectric. Contacts and the top gate patterned using the NanoFrazor lithography; b) Transfer curve of the FET from a) measured at room temperature and source-drain voltage $V_{\text{ds}} = 2$ V. $\text{SS} = 64$ mV per decade, $I_{\text{on}}/I_{\text{off}} = 5 \times 10^9$. The inset shows transfer curves at back-gate voltages from -20 V (yellow curve) to 20 V (blue curve). [5]

Surfactant-Free Sub-nanometric Copper Clusters. Synthesis, Characterization and Properties

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Sub-nanometric metal clusters formed only by tens of metal atoms and dimensions comparable to the Fermi wavelength of an electron, are attracting considerable attention during the last years. Due to the strong quantum effects, they exhibit unique and dramatic size-dependent properties such as photoluminescence, magnetism, circular dichroism, molecule-like energy gaps or catalytic activity, which makes them useful as building blocks to construct nano/micro structures with potential applications in fields such as biosensing, nanomedicine, nanoelectronics, catalysis, etc.

To date, the most of the chemical methods reported in the literature to prepare metal nanoclusters are based on the use of protecting ligands such as thiols, amides or phosphines. However, the presence of such stabilizing agents compromise most of the emergent applications of clusters such as catalysis. Kinetic control techniques [1] based on the use of electrochemical methods offer a very simplistic way to overcome these problems. By using such approach, Au and Ag nanoclusters in the range 2-10 atoms with enhanced catalytic [2] and biological activity [3] were already synthesized by our group without the needed to use any stabilizing and capping agent.

Among the metals, Cu is widely used in industry because of its high conductivity, similar properties to gold and silver and especially much lower cost [3]. However, due to the lack of efficient synthetic processes, reports about copper clusters are still scarce. Here, we present the recent advances in the synthesis of Cu sub-nanometric naked clusters less than 10 atoms by using a simple electrochemical method. The main effective reaction parameters (i.e. current density, voltage, electrode area, time reaction, and electrode roughness) affecting the cluster size and reaction kinetics will be discussed. Clusters were characterized by UV-Vis spectroscopy, Fluorescence Spectroscopy and Mass Spectroscopy.

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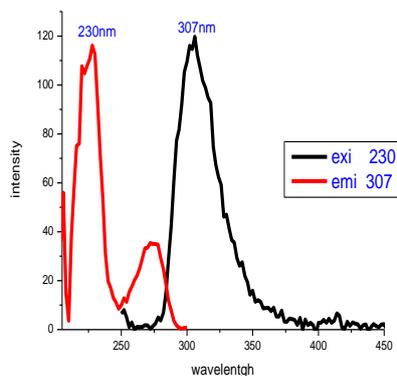


Figure 1: Fluorescence spectroscopy of Cu5 clusters

Single-Cell Probe Force studies to identify Sox2 overexpression-promoted Cell adhesion variations in MCF7 Breast Cancer Cells

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Replacement of the tip by a living cell as probing element in Atomic Force Microscopy (AFM) experiments permits direct quantification of cell-substrate and cell-cell adhesion forces. This is called Single-Cell Probe Force measurement technique [1]. When complemented with the use of optical/fluorescence microscopies it allows a controlled manipulation of the cell, and a well-defined location on the area of interest. In this work, a setup based on two glass-half-slides -a non-fouling one with bacterial S-layer protein SbpA from *L. sphaericus* CCM 2177, and a second half-slide with a fibronectin layer- has been employed to measure adhesion of MCF7 breast cancers, in two different states, towards fibronectin films (and SbpA as control) and cells (symmetric vs asymmetric systems). Measurements aimed at characterizing the adhesion behavior of Sox2 factor-overexpressing MCF7 cells, which are more invasive and of higher aggressiveness than control cells [2]. Together with the use of fluorescence techniques (epifluorescence, TIRF) the visualization of Vinculin and Actin distribution in both control MCF7 and Sox2-overexpressing cells in contact with fibronectin surfaces is enabled. Hence, the respective formation of adhesion complexes (i.e. focal adhesions) could be monitored and quantified. Results show the validity of

this combined approach for the comparison between cell lines.

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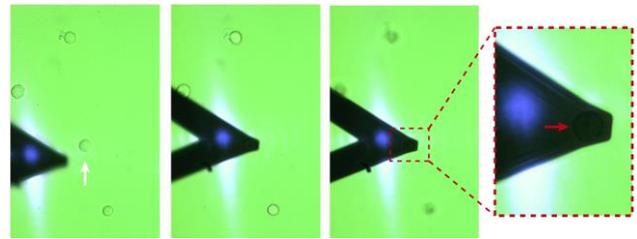


Figure 1: (left to right) Cell capture process sequence. The pre-modified tipless cantilever approaches the target cell (on a SbpA coating) until soft contact is achieved. Retraction after few minutes allows cell capture (see magnification).

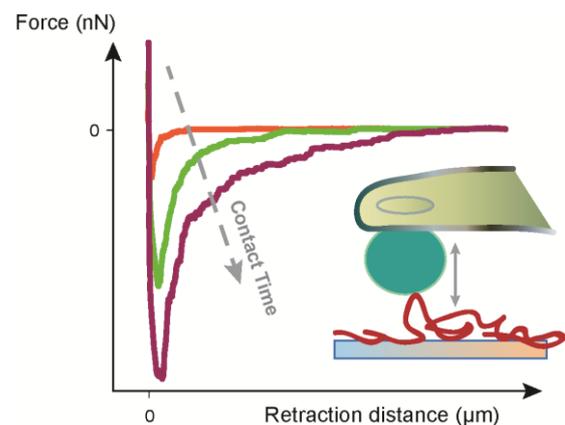


Figure 2: Schematic view of a cell-substrate interaction measurement, showing the corresponding contact time-dependent force vs distance plots at the retraction segment.

Analyzing the loading and release of Rhodamine 6G dye from Nanoporous anodic alumina rugates filters using optical methods

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Abstract

Porous materials constitute one of the best templates to be used in several drug delivery applications [1-2]. Amongst them, crucial developments have been reported in the field of widely known Nanoporous anodic alumina (NAA). Finely tuned engineering, along with ease of fabrication, stable optical signals, mechanically robustness and several reported chemistries on NAA have now made it easier to fabricate such structures [3-4]. On the other hand, reliable and effective drug release strategies need to be developed based on NAA for which it is an urgent requirement to understand in-depth loading and release mechanisms of several drug/dye molecules from the nanopores.

In this work, we have fabricated NAA-Gradient Index Filters (NAA-GIFs) platforms to gather information about the filling and release dynamics of Rhodamine 6G dye used as a model for a drug (Fig 1 a & b). Multiple photonic stopbands were designed in the structures being one in the absorption range of the dye while other one far from the absorption region. Simulations show (Fig. 2) that different amounts of dye inside the pores can be estimated by measuring the relative height of the maximum reflectance corresponding to the two stop bands. Reflectance measurements were also taken before and after dropping dye on the surface. Release profiles were measured by registering the change in reflectance spectra as the fluid wets the sample in a custom-made flow cell. All these results are put together to gain more information about the molecular behaviour inside the structure.

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Figures

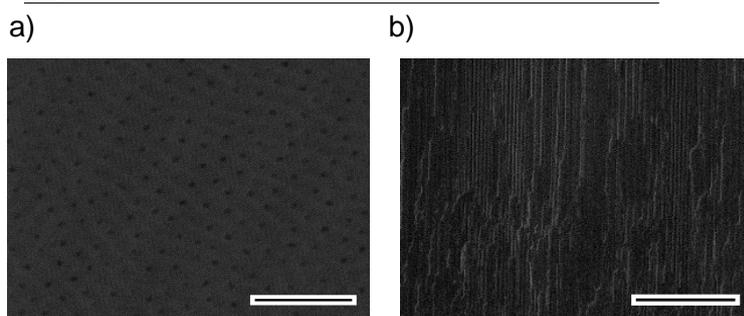


Figure 1: a & b) ESEM top and cross section of the NAA-GIFs respectively. Scale bar 1µm

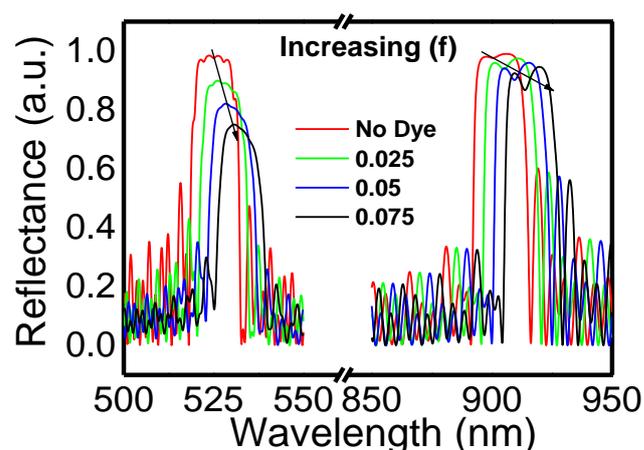


Figure 2: Simulation analysis of NAA/GIFs before and after dye filling inside nanoporous channels.

Highly effective gating of graphene on GaN nanopillars and epilayers

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In this communication we present results of highly effective graphene gating using GaN epilayers (EPI GaN) as well as vertically aligned GaN nanopillar structures (GaN NP). In the EPI GaN a 100 nm thick layer of undoped GaN preceded by a 3 μm thick layer of highly conductive GaN was grown on a sapphire substrate (Fig. 1a inset). 200 nm diameter thick GaN NP were etched in EPI GaN by plasma method [1]. Four-layer graphene (FLGr) was used as a top contact to the GaN structures. Current-voltage characteristics show Schottky-like characteristics for a reverse biased voltage up to -5 V in both samples (Fig. 1a). Raman spectra measured for these structures show a strong shift of the G band as a function of gate bias (Fig. 1b, c). In graphene on GaN NP a blueshift up to 1.4 cm^{-1} is observed while for graphene on EPI GaN a redshift of up to 9.6 cm^{-1} is present (Fig. 1d). Furthermore, the G band in graphene on EPI GaN clearly splits, which suggest different carrier concentrations of subsequent graphene layers in the FLGr structure (Fig. 1b). Our results suggest that graphene on EPI GaN is p-doped, while n-doping is characteristic for graphene on GaN NP. Interestingly, a substantial Raman shifts occurs in our Schottky diode structures at one order of magnitude smaller voltages than for graphene deposited on SiO₂ substrates in capacitor type devices [2]. These obtained gating efficiency is comparable to the results for solution-gated graphene. This strongly suggest that the diode junction is located directly near the graphene layers [3]. Thus, graphene gating is effective at very low voltages which is highly promising for further electron-phonon studies as well as possible applications like nano LEDs.

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FIGURES

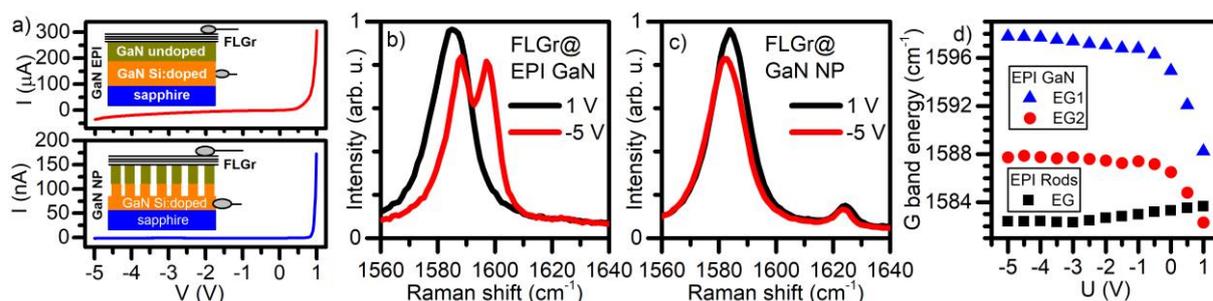


Figure 1: a) IV characteristics; insets present sample schemes. Graphene G band measured in samples: b) EPI GaN, c) GaN Rods, d) dependence of G band energy on diode voltage.

Strain-tunable Quantum Optical Emission in WSe₂ Monolayers

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Abstract

The development of novel ultra-compact two-dimensional (2D) photonic technologies for quantum information processing relies on our ability to fabricate single photon sources (SPS) in 2D van der Waals materials with controlled optical emission properties and on-demand¹. However, the efficient exploitation of such quantum emitters in quantum information science and technology requires an in-depth understanding of their physical origin and a deliberate control over their optical emission properties. In this regard, elastic strain engineering provides interesting possibilities. One of the most prominent experimental approaches to date for the introduction of controlled in-plane strain fields in nanomaterials is based on the use of a novel class of piezoelectric actuators^{2,3}.

In this work, we demonstrate reversible tuning of the emission energy of SPS in wrinkled WSe₂ monolayers upon their integration onto piezoelectric actuators capable of introducing in-plane isotropic and anisotropic strain fields⁴. Our findings demonstrate that it is possible to have a full control of the emission energy with a high energy shift up to 20 meV while leaving the single photon purity unaffected. Finite

element simulations suggest that the type of strain (tensile or compressive) experienced by the quantum emitters, i.e. red or blue emission energy shift, strongly depends on their localization across the wrinkles. Our findings shed light on the understanding of the physical origin of SPS in 2D monolayers and are of strong relevance for the practical implementation of single photon devices based on 2D materials as well as for understanding the effects of strain on their emission properties.

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Figures

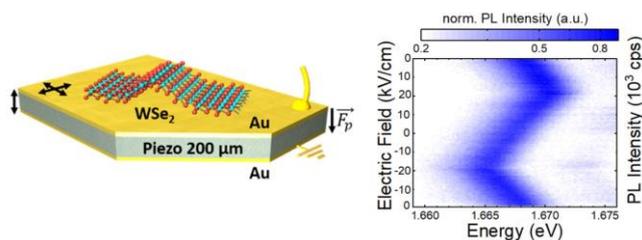


Figure 1: (Left) Schematics of a WSe₂ monolayer on a piezoelectric actuator to introduce reversible in-plane strain fields. (Right) Reversible and active tuning of the optical emission of single photon emitters.

Gold Nanoparticles Chemiresistors: towards e-tongues for Ions Sensing

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The combination of metal nanoparticles (NPs) with ad hoc supramolecular receptors of the analyte of choice represents a powerful strategy for the fabrication of novel hybrid plasmonic sensors.[1] On the one hand, AuNPs are ideal scaffolds because of their highest surface-to-volume ratio combined with their unique optical and electrical properties.[2] On the other hand, supramolecular recognition has proven to be key to the realization of sensors exhibiting detection limits down to ppm/ppb levels with fast response speed combined with unprecedented selectivity.[3]

Here, we have devised a novel chemiresistor (CR) capable to perform real-time sensing of ions. Such devices are based on the use of all-covalent 3D networks obtained by interconnecting AuNPs with dithiolated crown ethers which act as molecular linkers. In the present case, we have performed the layer-by-layer assembly of AuNPs mediated by dithiolated crown ethers on a substrate with photolithographically patterned electrodes. The ion adsorption/desorption into the AuNP-based network is pivotal for the final performance. Such interaction can determine a modification of the network's structure (e.g. via swelling) or electronic properties (e.g. via a change in the device resistance). The performance of such devices was studied and optimized in terms of NPs size as well as the geometry of the gold interdigitated electrodes. Finally, to demonstrate the sensing capabilities of

these hybrid nanocomposites we have performed the real time detection of potassium ions (K⁺) in water.

The ultimate goal is to develop a technology that can be implemented in portable optoelectronic devices, whose performance can compete with state-of-art devices within this field of interest.

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Spray Pyrolysis Technique Utilized for the Fabrication of Inverted Polymer Solar Cells

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Currently, polymer solar cells (PSCs) used for harnessing solar energy based on organic materials get more attention than silicone solar cells due to their lower weight, higher flexibility, lower manufacturing cost, short energy payback time as well as facile conjugation with other electronic applications [1]-[2].

Variety of thin film deposition techniques have been utilized for the fabrication of the PCs [3]-[4]. In our work, the fabricated PSCs have the inverted structure (iPSCs) as showed in Fig.1. In addition, the electron transporting layer used was ZnO which has been deposited by the lab-scale spin coating technique (ZnO-SC as a control cell) along with the spray pyrolysis technique (ZnO-SP as a case of investigation).

The obtained results in this research illustrated that both ZnO-SC and ZnO-SP have similar performance (10%) as demonstrated in Fig.2. But, the main advantages were not only high cells' performance but also the ability to fabricate the ZnO thin film with SP technique which is simple manufacturing process with low cost and reproducible technique [5]-[6]. Moreover, it can be promising technique to integrate the iPSCs for the industrial mass production scale as well as maintain the cells with efficient performance.

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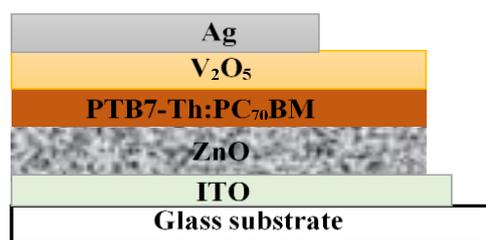


Figure 1: Structure of the Fabricated iPSC.

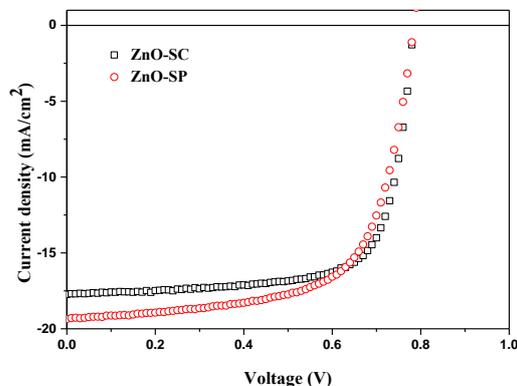


Figure 2: Current density - Voltage curve for ZnO-SC and ZnO-SP iPSCs.

Nanographene production scale-up and its biomedical applications with focus on cancer phototherapy

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Abstract

Cancer, the second leading cause of death worldwide, requires more effective treatment strategies. Photothermal therapy (PTT) is a non-invasive alternative based on the use of near infrared (NIR) light energy. It results in hyperthermia (39-47 °C), leading to increased membrane permeability, which, in turn, induces higher nanoparticle/drug uptake and consequent tumor cell apoptosis. Graphene-based materials (GBM), owing to their large surface area and strong radiation absorption, can act as platforms for chemo-photothermal therapy.

Through a simple and facile method functionalized rGOn was obtained as a promising photoabsorbing agent for PTT applications in non-melanoma skin cancer treatment. The combination of this functionalized nanomaterial with NIR irradiation using a safer LED-based NIR light source opens new possibilities toward exploring lower power and cheaper systems for mild hyperthermia cancer therapy, enabling better control over nanomaterial heating.

GBM have been studied regarding their biocompatibility; their lateral size, surface oxidation degree, and surface modification with polymers revealed to impact on biointeractions.

Recently, a system has been developed by our team, which allows the scale-up of water stable monolayer nanographene (<200nm) production. Smaller materials usually present better biocompatibility, penetration through skin and cell internalization.

GBM have been shown to provide mechanical reinforcement of polymers used for 3D printing of biomedical implants, preventing mechanical properties decay during hydrolytic degradation at body temperature.

Acknowledgements

This work was financed by FEDER funds through the COMPETE 2020 - Operacional Programme for Competitiveness and Internationalisation (POCI), Portugal 2020, and by national funds (PIDDAC) through FCT/MCTES in the framework of the project POCI-01-0145-FEDER-031143, and Base Funding - UIDB/00511/2020 of the Laboratory for Process Engineering, Environment, Biotechnology and Energy – LEPABE.

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Graphene nanosheets produced by a green liquid phase exfoliation process.

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Developed at the laboratory of geophysical and industrial flows (LEGI, University Grenoble Alpes), Grenoble Green Graphenofluids offers graphene nanosheets suspensions. Graphene nanosheets are exfoliated from graphite particles by an innovative microfluidic process using hydrodynamic cavitation 'on a chip' [1, 2]. The quality of exfoliated nanosheets is asserted by SEM, TEM, AFM and Raman analyses. GGG produces graphene nanosheets whose thickness runs from 1 to 10 carbon layers, with an average 150 – 300 nm lateral size. They are delivered in a solution at a concentration between 2g/L and 10 g/L. Exfoliation from aqueous solutions with surfactant, as well as from solvents with surface energy matching those of graphene, have been performed. Aqueous or solvent based suspensions use biodegradable dispersing agents, allowing GGG to be an environmentally compatible process in graphene production. Low hydraulic power is required, so that the low-cost mobile experimental facility is able to produce graphene nanosheets on demand, under the best possible conditions of safety. A review of the graphenofluids produced by such a process and of their intrinsic properties will be presented. We are looking for industrial partners to test the interest of our products for a large scope of applications.

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Figures

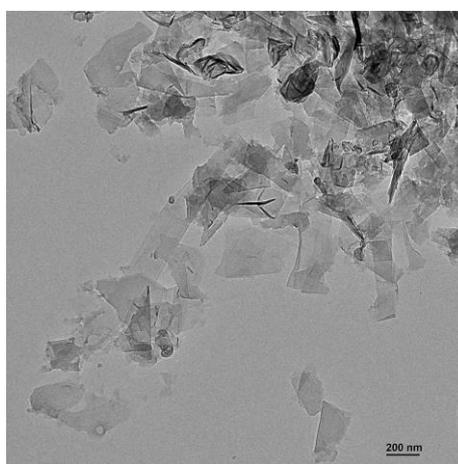


Figure 1: TEM observation of graphene nanosheets produced by GGG. The scale bar is 200 nm.

Fluorescence dye-silica nanoparticle for detection of cancer cells

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Cancer is the second cause of human death worldwide, and its early diagnosis is the key for an effective treatment. The most used imaging techniques, based on X-ray sources or high magnetic fields, can generate side effects in the patients. For that, fluorescence microscopy, a less invasive technique can be considered as a promising strategy to detect cancer cells by the use of suitable fluorophores. However, the most common fluorophores are not designed specifically for stain cancer cells and chemical modifications that increase the cost are required. On the other hand, the use of nanoparticles could be a more promising approach to overcome the fluorophores limitations. Mesoporous silica nanoparticles (MSN) have several benefits to be used as nanocarrier for bioimaging: high surface area, easy functionalization, good biocompatibility, optically transparent properties and low cost. [1]

In this work, mesoporous silica nanoparticles of monodisperse size distribution of around 50 nm are synthesized by modified Stöber method, Figure 1.[2] MSN was used as a carrier for a commercial dye, rhodamine 101 (R101), which was occluded inside the mesoporous of silica nanoparticles or anchored in their external surface.[3] Moreover, to ensure their good stability in water and their selectivity for cancer cells, polyethylene glycol chain and folic acid, respectively, were tethered in their external surface. As a result, well-dispersed silica nanoparticles with high fluorescence and good selectivity for cancer cells are obtained. Finally, in vitro experiments in HeLa cells were carried out to test their capability as biomarkers, Figure 1.

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FIGURES

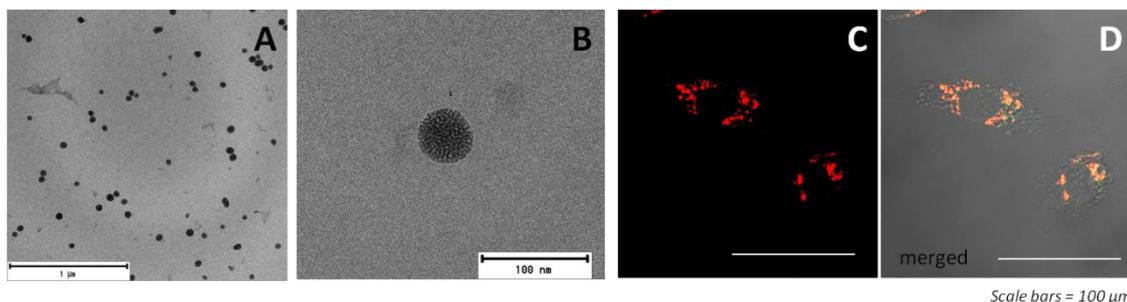


Figure 1: TEM image of mesoporous silica nanoparticles (A and B) and fluorescence images of R101-MSNs in HeLa cells at 1 μg/mL (C and D).

Electrochemical synthesis and characterization of silver atomic quantum clusters of three atoms

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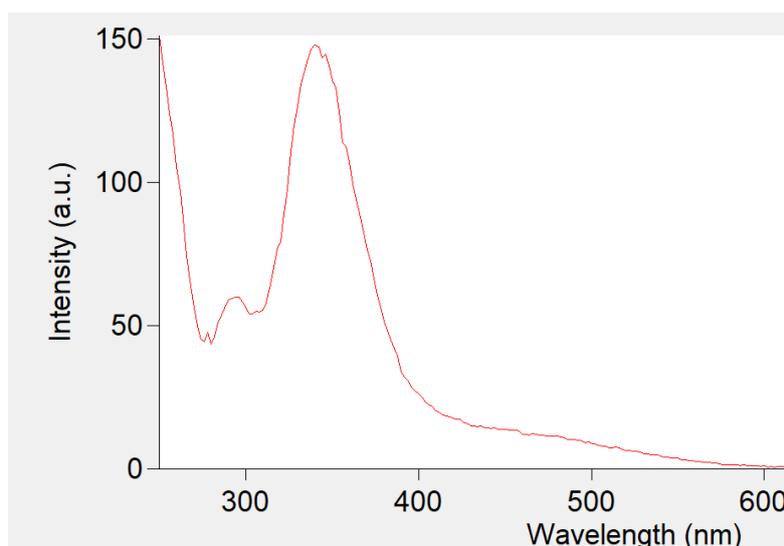
Atomic quantum clusters are materials formed by a small number of atoms, which give them unique properties due to quantum effects. The size of the clusters is less than one nanometer and they are totally different from the conventional nanoparticles and bulk metal. Besides, their properties strongly depend on the number of atoms making them very different from each other [1]. However, this great dependence on the cluster size, makes necessary the synthesis of very monodisperse clusters. This work presents the synthesis of silver clusters of 3 atoms, interesting due to their great properties on the therapeutic field, as they can improve the chemotherapy efficiency of classical antitumorals. [2]. Electrochemical synthesis is proposed in this case to obtain Ag₃ clusters, controlling different parameters such as time, temperature or applied potential to adjust the reaction kinetics -key point of cluster synthesis-[3] in order to get a highly monodisperse Ag₃. Furthermore, fluorescence spectroscopy is used to characterize the product. This technique is very useful in this case because it allows us to distinguish between the different cluster sizes by using the Jellium model. This study concludes testing the samples with the enzymatic activity of Hind III which confirms the Ag₃ presence.

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FIGURES

Figure 1: Fluorescence spectra of a silver three quantum cluster sample



ATOMIC QUANTUM CLUSTERS AS CATALYST OF ANTIRRADICAL REACTIONS

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The study of antirradical agents has been attracting great attention in the last years because free radicals are responsible of several serious diseases such as cancer growing, cataract, diabetes mellitus, rheumatoid arthritis and cardiovascular diseases. Besides, they are involved in polymer degradation with enormous practical consequences like the well-known autooxidation of hydrocarbons, considered in the case of feed lipid components as the major cause of reduction in feed quality, and also the reason of the inexorable deterioration of polymeric materials.

The 2,2-diphenyl-1-picrylhydrazyl (DPPH) is a stable radical widely studied in this kind of investigations because its easy characterization by UV-Visible spectroscopy and its high stability as a solid and in solution.

Atomic quantum clusters (AQC)s are new materials whose size is less than ≈ 1 nanometer. They have a molecular-type structure, being a bridge between atoms and nanoparticles. These new materials show novel and unexpected properties, completely different to those displayed by the bulk metal or in nanoparticles, such as catalysis, photoluminescence, biocompatibility...

In this short talk we show for the first time AQC)s, and more specifically silver 5 atoms clusters, acting as catalytic radical scavengers against the radical model DPPH.

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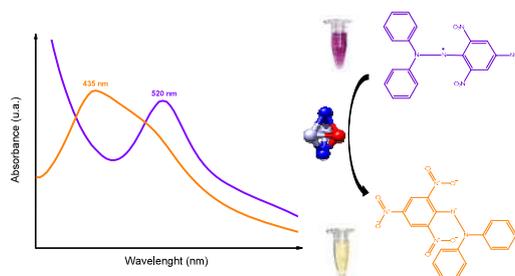


Figure 1: Reaction scheme and UV-Visible spectrum of the reduction of DPPH catalysed by Ag_5 -AQCs.

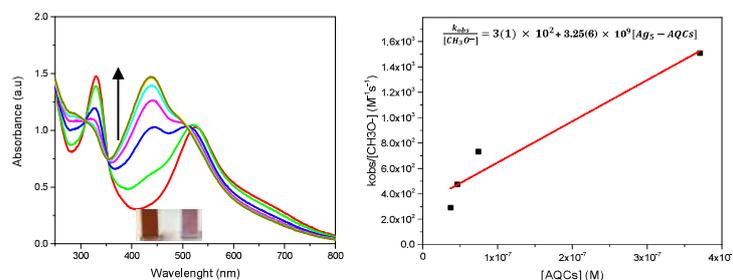


Figure 2: Changes with time in the UV-vis spectra of DPPH 1.125×10^{-4} M in the presence of $200 \mu\text{g/L}$ ($\approx 3.7 \times 10^{-7}$ M) Ag_5 -AQCs in methanol and the representation of the kinetic constant versus Ag_5 -AQCs concentration.

Nanopores as single-molecule tools in nanobiotechnology

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Abstract

A single nanometer wide aperture made in an electrically insulating membrane can be used as a single-molecule sensor by monitoring the ionic current flowing through the pore (Figure 1). The measurements are exquisitely sensitive, modulated by the atomic structure of the analyte at the lumen of the pore, and allow single-molecule DNA sequencing as a DNA strand translocates the nanopore in single-nucleotide steps.

Here I will show the research we are doing to analyse proteins [1] (Figure 2), manipulate proteins and, ultimately to sequence single-protein molecules [2]. We are also exploring the use of nanopores as single-molecule barcode readers [3] that, in addition to the barcode read provides and additional biophysical measure on the barcoded molecule of utility in drug-discovery and multiplexed diagnostics.

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Figures

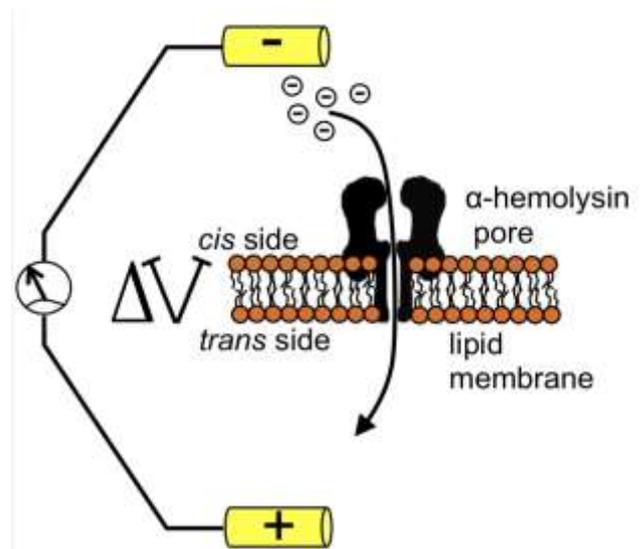


Figure 1: A single nanopore inserted in a lipid membrane allows the flow of ions in response to an applied electric potential. The ionic current can be measured with fine detail, and analytes detected if they decrease the current when threaded into the pore.

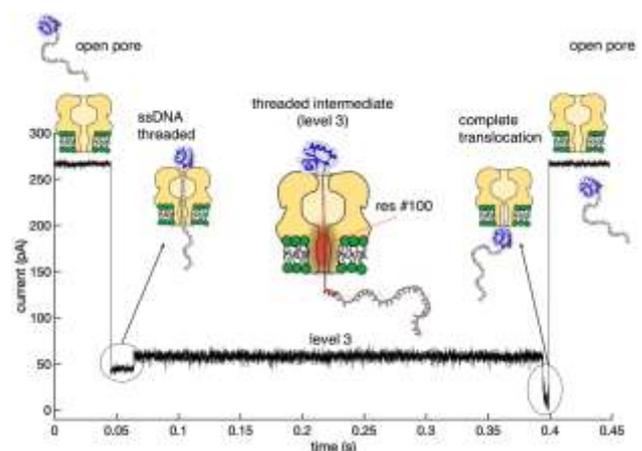


Figure 2: Ionic current signal obtained when a single protein molecule (blue) covalently attached to a ssDNA translocates a hemolysin membrane nanopore. The figures show the molecular structures associated to each step of the signal.

Algorithmic Detection of Oxide Nanosheets

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Oxide nanosheets with a wide bandgap have high dielectric properties, and they are single crystals delaminated by chemical exfoliation of bulk layered materials. These crystallites have an approximate thickness of 1 nm and a lateral size of up to 10 μm . The oxide nanosheets have demonstrated potential applications in a wide array of high-k dielectric [1], photocatalytic [2], photoluminescence [3], and p-n junction diode [4] applications. $\text{Ca}_2\text{Nb}_3\text{O}_{10}$ (CNO) nanosheets, a typical member of oxide nanosheets, have excellent dielectric properties due to their high dielectric performance related to $C = (\epsilon_r A) / d$. Thus, the thinner the dielectric layer in the capacitor composed of metal-dielectric-metal layers, the larger the capacity that can be stored. Therefore, it is necessary to use dielectric oxide nanosheets, having a thickness in the nanometer range.

A common method to detect oxide nanosheets is to use Atomic Force Microscopy (AFM) to scan the material, and manually locate them in the scanned image. Our preliminary study aims to automate this process with an algorithmic approach. Current studies focus on determining the thickness of other types of nanosheets [5, 6]. Our approach relies on the physical thickness of the CNO nanosheets while watching out for artefacts on an AFM image. Figure 1 displays the plot of a row from an AFM image (Figure 2, left). The image has artefacts such as stripe noises and intensity inhomogeneity (increased intensity along one diagonal in this case). For each row, we first detrend the signal to eliminate such

gradual intensity changes, remove outliers, use difference-based derivative estimation, so that the edges of potential nanosheets can be detected. As a result, we get the red markers in Figure 1, which are used as change points in the signal. We mark the pixels that are empirically close to the mean and have a low mean squared error. The resulting pixels are the nanosheets, as shown in Figure 2.

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Figures

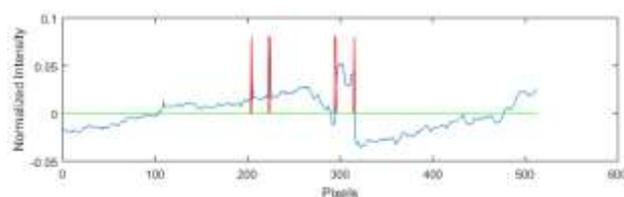


Figure 1: A normalised signal for a row in an AFM image, the detected change points are in red.



Figure 2: The oxide nanosheets on the left image are detected, as shown on the right.

Nanomed Spain, the Spanish Technological Platform for Nanomedicine: promoting public-private collaboration, innovation and clinical translation of nanomedicine in Spain

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Abstract

The Spanish Platform for Nanomedicine (NanoMed Spain - <http://nanomedspain.net/>) is a forum that brings together 170+ public research centres, hospitals, companies and government representatives active in nanomedicine. Nanomed Spain is an instrument to coordinate entities involved in research and innovation, fundamental to the transfer of results to industry and the health system in this highly multidisciplinary field. It is also a means of connection to facilitate the internationalization of initiatives and projects, with the aim of improving the competitiveness of Spain in this field. Industry in the biomedical and biotechnology sector plays a leading role in the Platform, very actively supported by technology centers, research organizations, universities and hospitals, as well as by the national public administration.

Nanomed Spain was created in 2005 based on the model of the European Technological Platforms and in particular, of the European Technology Platform on Nanomedicine (ETPN), also created in 2005 by the industrial partners of the area and the European Commission as a communication tool for all actors in the sector with the aim of contributing to the joint development of new and innovative medical products and applications.

The mission of Nanomed Spain is to promote and facilitate public-private partnerships in research and innovation in nanomedicine in Spain, with the aim of accelerating the development of innovative therapeutics and diagnostics based on the capabilities offered by nanotechnology applied to health care.

Over the past months, the important role of research and innovation and multidisciplinary and multisectoral collaboration has been stressed more than ever. In the fight against COVID-19, nanomedicine has proven to play a very important role. From diagnosis with the use of nanosensors to treatment with targeted therapies, through the design of vaccines using nanomaterials or the identification of new drugs through in vitro models of organoids.

It is necessary to continue advancing and generating knowledge in this field, as well as to continue working in the coordination of the healthcare sector with various industrial sectors (pharmaceutical, biotechnology, medical technologies) and research centers in order to face the new health challenges that may appear in the next few years in the most efficient way possible. In this talk we will review how Nanomed Spain contributes to this endeavor.

Promising artificial one-directional antenna system based on cyanine-doped hybrid material

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Although antenna systems can be found in nature, such as those responsible for photosynthesis processes, the synthesis and design of artificial antenna systems is not an easy task. The key factor is the mimicry of light-harvesting and sequential transfer that takes place in natural antenna systems, involving donor and acceptor molecules, usually chromophores [1]. In this work, artificial antenna systems consisting on different chromophores or different species of the same chromophore, in situ encapsulated into 1-D nanochannelled magnesium-aluminophosphates (MgAPOs) are synthesized and characterized. Through the crystallization inclusion method approach, the encapsulation of the dyes is not only performed in a unique step, but also a strategic distribution of the dye species along the nanochannels of the host is achieved (Figure 1), enabling one-directional Försters Resonance Energy Transfer processes between dyes or dye species absorbing and emitting light in different ranges of the electromagnetic spectrum. In this work, different hybrid materials are presented, prepared following this strategy, beginning with particles doped with pyronin Y (PY) and/or acridine (AC) [2,3], and reaching more efficient and long-range antennas incorporating a cyanine dye (PIC), appealing due to the intriguing properties of its J-aggregates [4]. The energy transfer in these materials has now been experimentally evidenced by remote excitation microscopy technique, resulting in the last case in an energy transfer reaching over tens of microns (Figure 2) [4].

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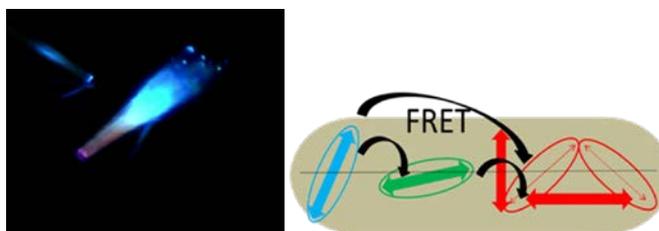


Figure 1: Left: fluorescence image of an AC/PY doped MgAPO-36 needle bouquet under UV excitation light. Right: Scheme of the energy transfer taking place in the system.



Figure 2: Fluorescence intensity image of a PIC/MgAPO-36 particle. 488 nm excitation was fixed at position pointed with an arrow.

Nanolayered MoS₂-Based Catalysts: A Convenient Choice for the Synthesis of Fine Chemicals

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Transition metal sulfides constitute a wide family of materials with many interesting applications in different research areas. In catalysis, cobalt (or nickel)-promoted MoS₂ materials have been extensively used as hydrotreating catalysts in petroleum refineries for upgrading crude feedstocks.[1] Nevertheless, the full potential of these materials, and in particular their application for selective transformations in fine chemistry, has been overlooked by the scientific community. Herein, it is shown that under fine-tuning modification they become in highly active and selective heterogeneous catalysts able to carry out hydrogenation and hydrogen-autotransfer processes in an efficient way directed to the preparation of valuable organic chemicals. More specifically, we have prepared a series of nanostructured cobalt-molybdenum sulfide based-materials by a one-pot hydrothermal synthesis, which furnishes the obtained unsupported catalysts with a high number of active sites per unit volume. As shown in Figure 1, they have been applied as catalysts for the chemo- and regioselective hydrogenation of nitro- and *N*-heteroarenes, as well as for the efficient C-S bond formation by reaction of alcohols with thiols.[2-4] An extensive characterization of the prepared nanostructured materials reveals their different composition, and how they undergo a continuing evolution during catalysis. Active phases responsible for the outstanding activity, chemo- and regioselectivity of these catalysts have been well-established.

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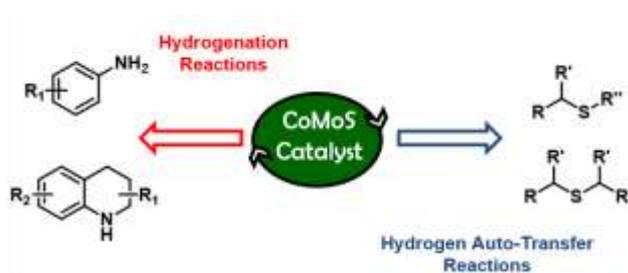


Figure 1: CoMoS-Catalyzed (Transfer-) Hydrogenation Reactions

Nano-scale temperature measurements using anisotropy-based nanothermometers for cancer theranostics

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Temperature is a crucial parameter in biology, medicine, and physics. Because of that, in the last years, several methods have been developed and presented to measure nanoscale temperature. Optical methods excel because they are non-invasive, spatially accurate and can measure real-time local changes in temperature. Among these, fluorescence anisotropy-based methods are particularly advantageous because they are less affected by changes in the probe concentration and irradiation conditions. Here we present intracellular temperature measurements in cancer cells and live organism using the green fluorescent protein (1,2) and a method to add thermosensitivity to any protein thereby transforming them into nanothermoters (3). The method consists of covalently attaching a dye to the protein, which increases the rotational time of the dye-protein system compared to the free dye, and confers thermosensitivity to the resulting bioconjugates. With this method, we transformed bovine serum albumin, glucose oxidase and catalase into nanothermoters. This also allowed us to analyze the anisotropy signal changes occurring during the catalytic cycle of catalase, as well as their correlation with the reaction exothermicity. In addition, it will also be presented the theoretical model that predicts the optimal sensitivity for anisotropy-based thermometers based on protein size and dye fluorescence lifetime (4). Using this model, most of the proteins and dyes can be converted to nanothermometers. The utilization of these nanothermometers by a broad spectrum of disciplines within the scientific community will

bring new knowledge and understanding that today remains unavailable with current techniques.

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Highly Selective, Non-Covalent Functionalization of MoS₂ – Inorganic-Organic Heterostructures

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Abstract

Transition metal dichalcogenides (TMDs) represent a class of layered, two-dimensional (2D) van der Waals materials, exhibiting a broad variety of electronic, optical and mechanical properties.

Controlling and modifying these by non-covalent functionalization with organic molecules became a major tool to tailor the materials surface chemistry and reactivity.

Merging the fields of organics and 2D TMDs can potentially induce charge transfer doping, resulting in tunable electrical properties in the heterostructures, which can be exploited in electrical devices such as diodes, FETs, chemiresistors or ChemFETs.

In this contribution the formation of self-assembled monolayers on monolayer, chemical vapour deposited (CVD) MoS₂ from physisorbed polycyclic perylene Bisimide (PBI) dendrimers, forming surface functionalized MoS₂ or molecule-encapsulated structures, is described. The high selectivity of this functionalization route is further demonstrated with time-of-flight secondary ion mass spectrometry (TOF-SIMS) and combined infrared atomic force microscopy (AFM-IR) with resolutions beyond the optical resolution limit. The potential of

hybrid inorganic-organic structures is shown within this study, giving rise to possible electronic and optoelectronic applications.

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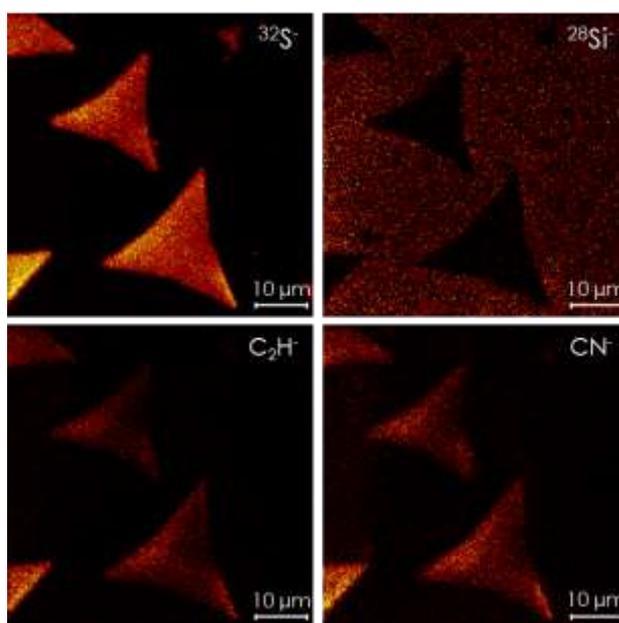


Figure 1: High-resolution TOF-SIMS maps of ³²S⁻, ²⁸Si⁻, CH₂⁻, and CN⁻ ions showing the planar distribution of the main elemental species on the surface of PBI functionalized MoS₂ on SiO₂. The CH₂⁻ and CN⁻ signals correspond to the PBI molecule, selectively deposited on the MoS₂ flake, represented by ³²S⁻ in contrast to the surrounding substrate, represented by ²⁸Si⁻ ions.

High-Performance Organic Photovoltaic Cells for Indoor Light Energy Harvesting

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Abstract

Organic photovoltaic (OPV) cells have attracted renewed interest for indoor energy harvesting because they can provide reliable and sustainable energy source for low power consumption electronic devices such as the rapid growth of Internet of Things. In this work, a high performance OPV under AM 1.5G illumination with a power conversion efficiency (PCE) of up to 10% are illuminated under indoor light source of commercial LED lamp with different light intensities. A strong dependency of the OPV performance with the illumination level is revealed by the optical and electrical characterization. As a result, the PCE of the devices illuminated under LED light is skyrocketed of up to 50% higher than those of OPV devices illuminated under 1 sun condition. The results suggest that OPV is an excellent candidate as a future dim-light power sources for the indoor application.

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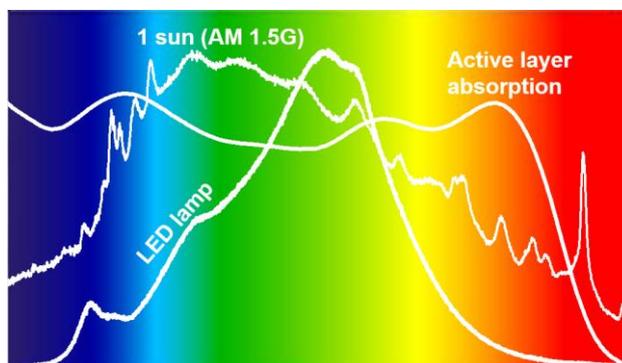


Figure 1: The spectra of AM 1.5G illumination (1 sun condition), LED lamp illumination (indoor light) and the active layer materials absorption.

● POSTERS

Development of magnetic nanocarriers for enhanced anticancer potential of lactoferrin

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Nowadays, the conventional drug administration faces several limitations that can be overcome by the development of multifunctional nanocarriers, such as the magnetoliposomes. These nanocarriers are composed of an aqueous core of magnetic nanoparticles (aqueous magnetoliposomes) or a magnetic core covered by a lipid layer (solid magnetoliposomes) [1]. These systems were chosen as carriers for lactoferrin, a protein that has been associated with anticancer activity [2]. In this work, both lactoferrin-loaded aqueous and solid magnetoliposomes were developed and characterized. Their biological activity, as well as the cellular uptake, were assessed in non-tumorigenic and in breast cancer cell lines. It was demonstrated that these nanosystems are cytocompatible for the non-tumorigenic cell line and cellular internalization occurs in both cell lines. The results show that magnetoliposomes are promising nanocarriers for proteins like lactoferrin, allowing its selective targeting and opening the possibility of a synergistic effect between this protein and antitumor drugs, together with enhanced cancer cell death by magnetic hyperthermia.

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Figures

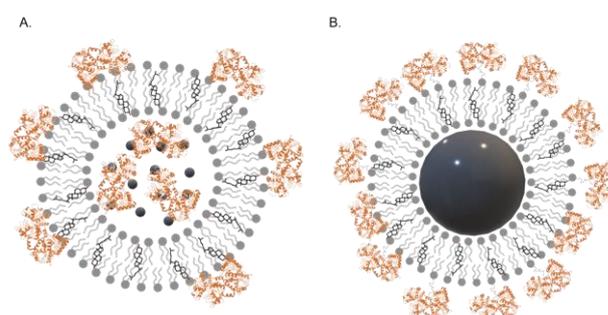


Figure 1: Schematic representation of lactoferrin-loaded aqueous (A) and solid magnetoliposomes (B). Magnetoliposomes contain manganese ferrite nanoparticles entrapped or covered by a lipid bilayer of egg phosphatidylcholine and cholesterol (7:3).

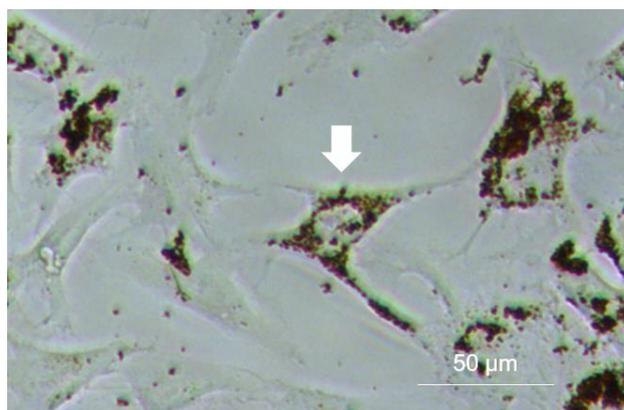


Figure 2: Bright-field photomicrography of cellular uptake of unloaded AMLs using *in vitro* breast cancer cells (Hs 578T). The white arrow evidences the presence of manganese ferrite nanoparticles inside the cells cytoplasm.

Metasurface configuration for selective infrared radiation source

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Abstract

Our objective is to develop IR sources with high emissivity control based on a narrow band absorber. The emission control is achieved by placing a metasurface tailored to attain nearly 100% narrow-band absorption at desired wavelengths.

Metasurfaces are periodic arrays of metallic or dielectric subwavelength structures of various shapes and sizes with geometrically controlled electromagnetic characteristics [1]. These structures have the potential to control both the propagation and the emission of light at the micro or nanoscale and have found applications in holography, sensors, switches, high-resolution imaging [2-4].

We propose a metasurface consisting of an array of circular-shaped metallic resonators (figure 1a) with diameter in the order of micrometres. The role of this configuration is to improve the light absorption within a narrow band interval in the IR domain. The metasurface is patterned on top of a classical thermal source (figure 1b) consisting of a metallic resistor.

The specifically tailored metasurface, placed directly over the heater, absorbs all the radiation spectrum emitted and will emit only the wavelengths for which it is designed. Figure 2a presents a SEM image of the fabricated metasurface, and figure 2b shows an optical image of the resistor used as thermal classical IR source.

Figures

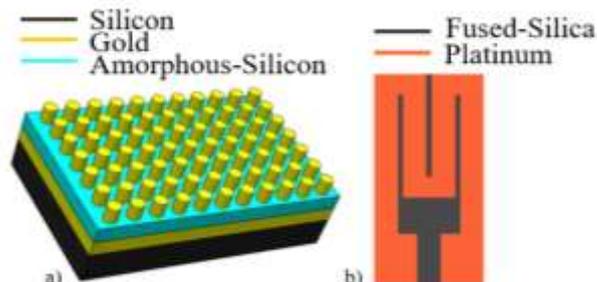


Figure 1: Thermal radiation source composed of: a) metasurface with tailored IR absorption spectrum and b) resistor based on meanders

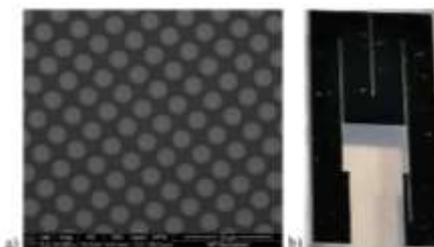


Figure 2: a) SEM image of the proposed metasurface and b) optical image of the resistor consists of two meanders

We designed and fabricated metasurfaces for IR sources with emissivity centred at $3.7\mu\text{m}$ and $5.4\mu\text{m}$ wavelengths suitable for gas sensing applications.

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Electromechanical properties of piezoresistive polymer materials as a function of the matrix and nanofiller content

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Thermoplastics and thermoplastic elastomers can be combined with different nanocarbon fillers for the development of piezoresistive composites with varying deformation ranges for sensing applications[1]. This work reports on the influence of the polymer matrix on the mechanical and electromechanical properties of polymer composites prepared by solvent casting. Nano carbonaceous filler such as CNT with varying contents up to 5 wt% were dispersed in polymer matrices of different mechanical characteristics, including poly(vinylidene fluoride) (PVDF), styrene-*b*-(ethylene-co-butylene)-*b*-styrene (SEBS) and thermoplastic polyurethane (TPU). The electrical properties of the composites are strongly related with the nature of the matrix. Piezoresistive sensibility in 4-point-bending and pressure modes is the largest for PVDF composites with filler concentrations around the percolation threshold: $GF \approx 2.8$ and $PS \approx 12 \text{ MPa}^{-1}$, at low deformation bending and pressure tests, respectively.

The different materials have been successfully implemented as pressure sensing materials for human walking

detection, allowing to compare the functional performance of the different polymer composite materials[2].

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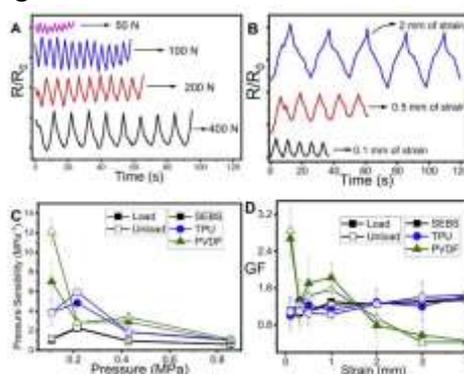


Figure 1: Piezoresistive response of PVDF, TPU and SEBS polymer composites with 5 wt% CNT, measured under uniaxial pressure.



Figure 2: Schematic representation of the developed prototype for walking detection based on piezoresistive surfaces.

Macro-scale contactless characterisation of graphene-based transparent electrodes

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Graphene is attracting a huge interest as promising candidate for the next generation of transparent electrodes (TEs) for applications such as displays, touch screens and/or solar cells [1]. In particular, graphene has outstanding properties to improve the energy-generation devices. In the context of photovoltaic (PV) technology, the implementation of graphene into new TE's architectures for silicon-heterojunction (SHJ) solar cells could offer innovative and low-temperature reliable solutions to generate and extract current in a more efficient way [2]. However, before graphene reaches an industrial production scenario, it is necessary to solve the bottleneck on how a quality control, that permits analysing large areas without damaging it, will be carried out. With this scope, this work presents two mapping procedures to characterising in an efficient macro-scale and non-destructive way, graphene-based structures; more specifically, TEs for SHJ solar cells. Those contactless mapping methods would permit the evaluation of the most important key performance indicators of graphene-based structures and their suitability for a specific application. They would also be very useful to extract information about both the uniformity and the quality of graphene-transfer process. Onyx system from Das Nano company, operating in reflection-mode at Terahertz (THz) wave range, and an optical-

transmission-mapping system developed by the authors, have been used successfully to determine the electrical and optical TEs performance, respectively, without damaging the graphene [3]. As example, Figure 1 pictures THz-time domain spectroscopy (TDS) conductance and resistance maps, acquired with Onyx, of an optimised TE based on three graphene monolayers transferred on the conventional transparent conductor oxide material, indium tin oxide (ITO), developed for SHJ solar cell technology.

We demonstrate that the use of such approaches allows opening new horizons to achieve the definitive take-off of graphene-based technologies, and specifically of their engagement in the SHJ contact-technology enhancement.

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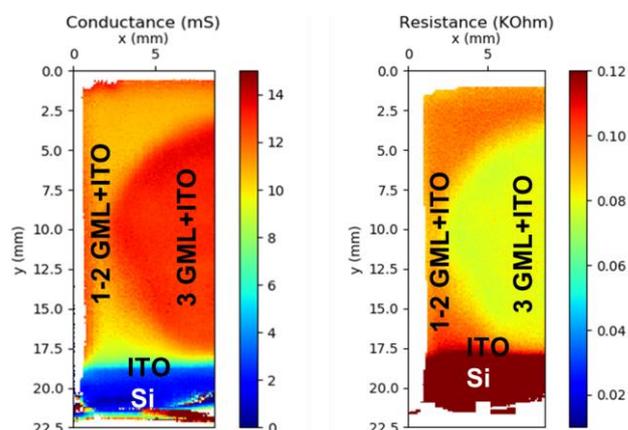


Figure 1: THz-TDS conductance and resistance maps of graphene-based TE acquired with Onyx

Acknowledgements: Supported by MINECO project DIGRAFEN (ENE2017-88065-C1-2R) and (ENE2017-88065-C2-2R)

Polymeric nanoparticle dispersions based on sustainable alternatives cosolvents to NMP

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Aqueous polymeric nanodispersions are real alternatives to reduce volatile organic compounds emissions in coatings and adhesive products. Aqueous polyurethane dispersions (PUD) have particular importance due to their similar performance to conventional solvent borne products[1].

This kind of dispersions are based on linear polyurethane dispersed in water due to an ionic internal emulsifier introduced in their molecular structure. The industrial fabrication process requires an organic solvent to reduce the viscosity during prepolymer synthesis. This organic solvent remains in the dispersion in order to allow coalescence of nanoparticles and film formation[2]. In industrial scale the solvent with better balance between performance and cost is N-methylpyrrolidone (NMP). However, the use of this chemical has been restricted by European Union [3].

In this study alternative green solvents have been selected and studied in order to get aqueous polyurethane nanodispersion with low toxicity and low carbon footprint [4].

NMP and three green alternatives have been used to synthesize PUDs following the same procedure in four cases. The dispersions obtained have been studied and compared, analysing: nanoparticles size distribution, Z- potential (electrostatic stabilization), stability time, figure e2 and polymer molecular weight.

According with all results obtained, the three sustainable alternatives to NMP studied are very promising for obtaining less toxic and more sustainable aqueous polyurethane dispersions. However, further

studies and researches are needed in order to validate these new sustainable solvents as substitutes of NMP in polyurethane nanodispersion systems.

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Figures

Solvent	Boiling point(°C)	Incineration	Recycling	Biotreatment	Aquatic impact	Air impact	Health Hazard	Exposure potential	Reactivity & Stability
NMP	202	3	4	3	10	6	1	9	9
1	203	4	4	5	9	6	4	8	10
2	207	8	7	10	10	6	4	8	10
3	242	4	5	6	10	10	10	10	10

Figure 1: Table. Scoring outcomes for solvents studied, GKS's sustainability guide: 1 the least green and 10 the most green [4].

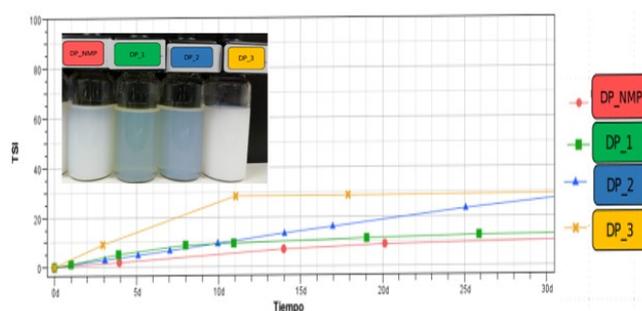


Figure 2: Nanodispersions photograph and graphic of destabilization kinetics

Cellulose nanocrystal-based hybrid films and aerogels

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Abstract

Naturally available materials like cellulose nanocrystals (CNCs) have attracted great interest during last years, owing to their low density, high specific surface, biodegradability, abundancy, high functionalization possibilities and vast applicability.

CNCs can be transformed into different structures including films, hydrogels, foams or aerogels with their particularities and application fields. To improve the functionality of CNC-based nanocomposites properties like mechanical resistance or thermal stability need to be analysed and modified through several alternatives.

In this work, cellulose nanocrystal based nanopapers and hybrid aerogels have been synthesized by evaporation-induced self-assembly (EISA) and freeze-drying techniques respectively. These materials have been reinforced using metallic nanoparticles or metal precursor. Samples have been analysed and compared to observe and explain changes in thermal stability, UV-Visible transmittance, wettability or antimicrobial activity.

Additionally, we were able to fabricate tougher aerogels through crosslinking CNCs with alginate biopolymer.

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Figures



Figure 1. Image of a cellulose nanocrystal-based aerogel

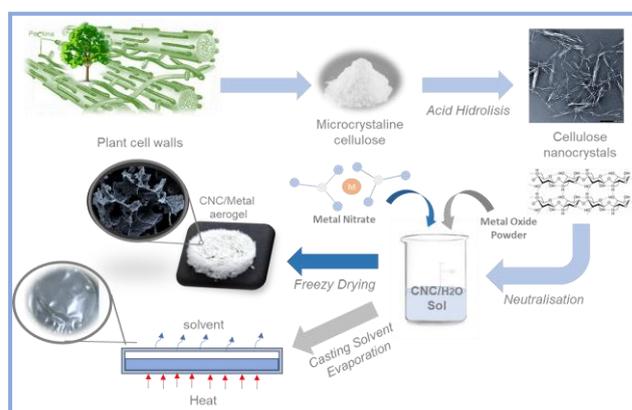


Figure 2: Illustration of the synthesis of CNC/metal nanocomposites

Colour characteristics of nanocrystalline WO_{3-x} thin films as a function of their stoichiometry

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Stoichiometric WO_3 crystallizes in tetragonal or hexagonal structures based on corner-sharing WO_6 octahedra. Each W ion is surrounded by six O ions, ideally forming an octahedron; whereas each O ion is bound to two W ions in a linear configuration, which can be represented as $\text{W}^{6+}-\text{O}^{2-}-\text{W}^{6+}$ [1]. One may assume that the basic building blocks are similar in the amorphous material, although bond lengths and bond angles exhibit considerable disorder.

Although stoichiometric WO_3 is a transparent oxide, there exist a number of sub-stoichiometric forms (WO_{3-x}) that exhibit different colours, ranging from blue in the case of a slight oxygen deficiency to brownish for WO_2 [2]. For the sub-stoichiometric oxides, the most common defects are the oxygen vacancies, which can be neutral (V_{O}^0), singly charged (V_{O}^+), or doubly charged (V_{O}^{2+}) with respect to the unperturbed lattice. The formation of a doubly charged vacancy and two W^{5+} ions seems to be energetically advantageous [3]. Thus, absorption of light can arise from the phonon-mediated excitation of an electron in one such W^{5+} site to a neighbouring W^{6+} site [3, 4].

In the present work, nanocrystalline WO_{3-x} thin films have been obtained by reactive sputtering of a metallic target (99.9% purity) on unheated glass substrates. The oxygen to argon partial pressure ratio (O_{pp}) has been changed to analyse its influence on the structural, optical and electrical properties of the samples. The main objective is to optimize their colour characteristics for smart windows and other related applications [4, 5].

Figure 1 shows the evolution of the optical transmittance of the sputtered films as a function of the O_{pp} . In parallel, the free carrier concentration is found increasing as the visible transmittance decreases. Then, the contribution of plasmonic absorption by free electrons has also been considered.

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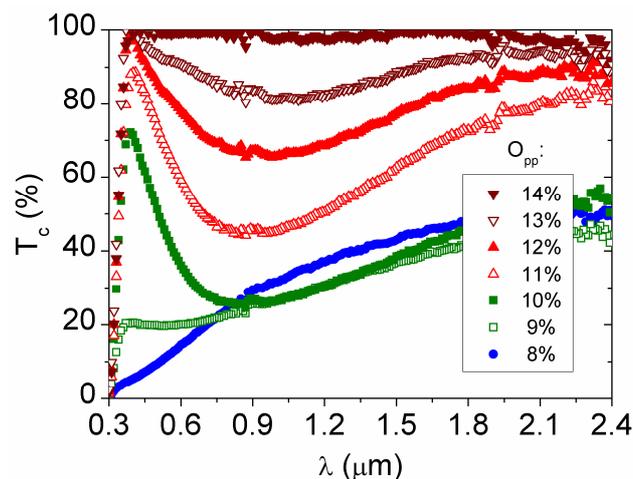


Figure 1: Optical transmittance of WO_{3-x} thin films prepared by reactive sputtering at different oxygen partial pressures (O_{pp})

LIPUS Activation of Gold Nanoparticle Anticancer Drug Carriers for Cancer Treatment

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With more than 10 million new cases of cancer predicted every year, there is significant motivation for the development of more efficient and accurate anticancer drugs [1]. When using conventional anticancer drugs healthy cells are often killed along with tumour cells, causing toxicity to the patient. Ultimately, this can limit the achievable dose to tumour cells, as well as patient outcome [1]. To overcome this limitation a number of anticancer drug delivery systems have been proposed, with one attractive method being that of nanoparticle drug delivery. Nanoparticle drug carriers can offer a number of advantages, including: the efficient delivery of lipophilic drugs, protection from aggressive environments, and both targeted and controlled drug delivery [2]. In this work the advantages of nanoparticle drug carriers and natural anticancer drugs, such as curcumin [3], were combined in a drug delivery system. Furthermore, active targeting was achieved by inducing anticancer drug release noninvasively via therapeutic low-intensity pulsed ultrasound (LIPUS) activation; either through mechanical stimulation or bulk heating of a region of interest such as a tumour. Gold nanoparticles (GNPs) were selected as anticancer drug carriers due to their inertness and high surface to volume ratio. Additionally, gold compounds have been shown to inhibit proliferation and cause cell cycle arrest in tumour cells [4]. GNPs in particular have also been shown to play a role in mediating anti-cancer activity, and improving uptake of chemotherapeutic drugs into tumour cells [5]. In order to

model anticancer drug release, a numerical COMSOL[®] based model of LIPUS activated anticancer drug release from GNP drug carriers was developed. Through simulating drug release for a variety of LIPUS and GNP parameters, the mechanisms of action behind ultrasound-nanoparticle interactions can be studied, and an optimized set of LIPUS exposure and GNP parameters can be determined. These parameters can then be applied experimentally to achieve efficient LIPUS induced targeted anticancer drug release from GNP drug carriers in *ex vivo* and *in vivo* tissue models.

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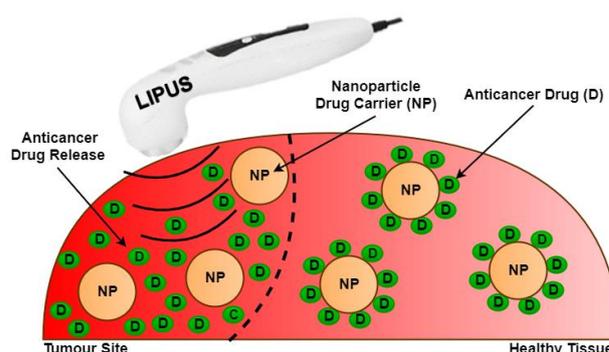


Figure 1: LIPUS activated targeted anticancer drug release from GNP drug carriers. Here anticancer drug release can be achieved at the tumour site, while sparing healthy tissue.

Development of Gold Nanoparticles of Various Morphologies for Targeted Drug Delivery

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Combining advantages of nanotechnology with anticancer drugs represents an efficient, logical and alternative approach for cancer treatment [1]. Targeted drug delivery is already an emerging topic and it's all set to be the next generation of drug delivery agents. Meanwhile it has been recently discovered that natural molecules like curcumin, etc. have anti-cancer properties [2]. In this aspect we have combined the advantages of both nanotechnology and drug molecules to develop novel nanodrug delivery systems where ultrasound waves will trigger the drug release from the surface of nanoparticles. As a carrier we have chosen gold nanoparticles which have properties like inertness, high surface to volume ratio and low toxicity. We have developed a one pot green method for the synthesis of gold nanocrystals in presence of trisodium citrate which does not require mechanical stirring, organic solvents or high temperatures. The process involves reducing gold salt by trisodium citrate at room temperature in presence of a third molecule like L-tyrosine, drug molecules, polymers like polyvinylpyrrolidone (PVP) or dyes like fluorescein isothiocyanate (FITC) which resulted in a colloidal sol after few hours of reaction[3,4]. The morphology of final nanoparticles depends on the type and amount of additional molecule added with citrate. For example, with L-tyrosine the final colloidal sol is either blue or red in colour depending on the sequence of addition of reagents. The blue colour was due to formation of nanoflowers while red colour was due to formation of quasi spherical shape. In presence of PVP or FITC a bright

red colour was developed indicating spherical shape. Electron microscopy images of nanoparticles synthesized in presence of PVP indicated ultra-small spherical particles with size of less than 5 nm. Additionally, this sol was extremely stable and did not precipitate even at high salt concentration or cell culture medium. Another additional feature of this method is that the citrate molecules also act as a base for the attachment of additional molecules like 11-mercaptoundecanoic acid (MUA) and enzymes like glucose oxidase (GOx) [4]. The particles are purified by centrifugation to remove any free unreacted reactants.

Moreover, as part of this project, the release of anti-cancer drugs from the surface of gold nanoparticles by ultrasonic waves are investigated. The developed gold nano-delivery system will be tested in targeted treatment of cancer tumours.

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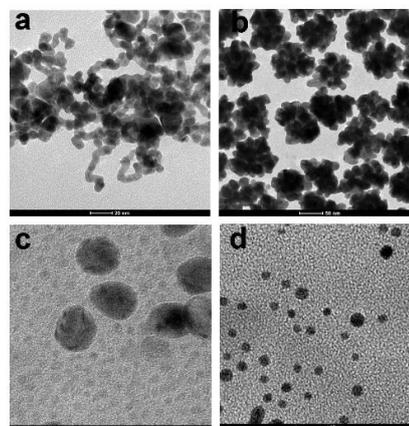


Figure 1: Gold nanoparticles synthesized at room temperature in presence of (a) Citrate, (b), c) citrate & L-tyrosine (d) Citrate & PVP.

Selective lectin multimodal biosensing on functionalized graphene

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Abstract

Graphene has a wide potential for applications in biotechnology such as selective biosensor due to its electronic properties and strict monolayer character. However, the outstanding sensitivity is compensated by null inherent selectivity, which must be introduced by secondary processing, such as chemical functionalization. Using a reaction sequence, we were able to covalently graft carbohydrates moieties onto graphene. Reaction with gaseous XeF₂ introduces C-F defects in the structure, which are smoothly exchanged for strong nucleophiles, such as propargylamine. The triple bond can be then used in CuAAC reaction with azide-terminated N-acetylglucosamine (GlcNAc) oligomers to tether these carbohydrates onto the monolayer. GlcNAc oligomers bind lectins specifically and reversibly. We investigate the affinity of on-surface grafted glucosamines of different length towards lectins (WGA, *Triticum vulgare*). In the experiments we use mono- to penta-GlcNAc and evaluate the strength of binding by competitive series. The GlcNAc-grafted graphene can be used as a selective active layer of lectin sensors using spectroscopic, microscopic, electrical or mass detection.

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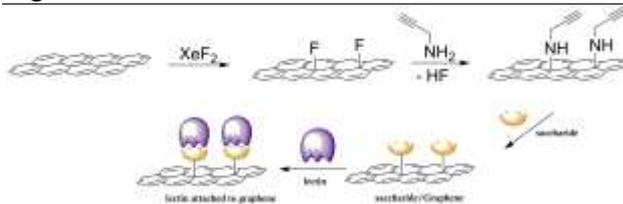


Figure 1: Functionalization of graphene, covalent grafting of carbohydrates and selective binding of WGA.

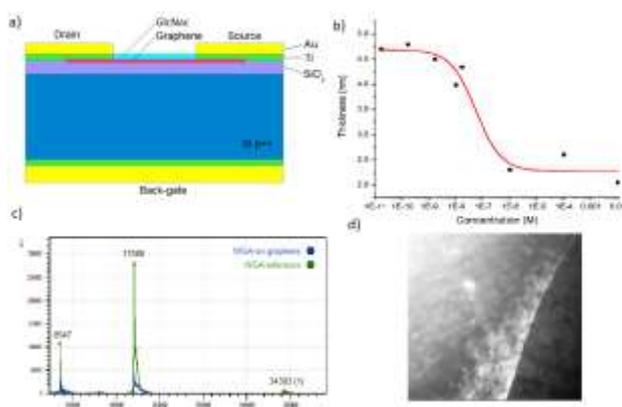


Figure 2: Modes of detection using the GlcNAc functionalized graphene: a) GFET configuration for electrical detection, b) microscopic detection by AFM, c) mass spectrometry, d) fluorescent measurement/imaging.

Hydrogenation of CO₂ on iron-based catalysts

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Nowadays, global warming represents significant ecological problem. The crucial aspect is the increasing concentration of greenhouse gases (especially CO₂) in the atmosphere. [1] Possible solution could be assigned to the lowering concentration of CO₂ by conversion into more valuable compounds. [2] For this purposes, iron-based materials demonstrate one of the most effective catalytic material for CO₂ hydrogenation to methane, methanol and another simple hydrocarbons. [3]

This study focuses on catalytic hydrogenation of CO₂ in the gas phase. The reactions proceed at low pressure of 1 bar and the temperature of 325 °C on the catalysts. These catalysts are prepared samples of mesoporous iron oxides with a high surface area. All prepared catalysts are produced CH₄ by conversion unlike the commercial Fe₂O₃ used as reference. By-products of reactions are CO and H₂O. The catalytic activity is different for each sample and relates to a presence of Fe₃C phase in prepared catalysts.

The authors gratefully acknowledge the support provided by the Internal Grant of Palacký university in Olomouc - IGA_PrF_2019_033.

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Figures

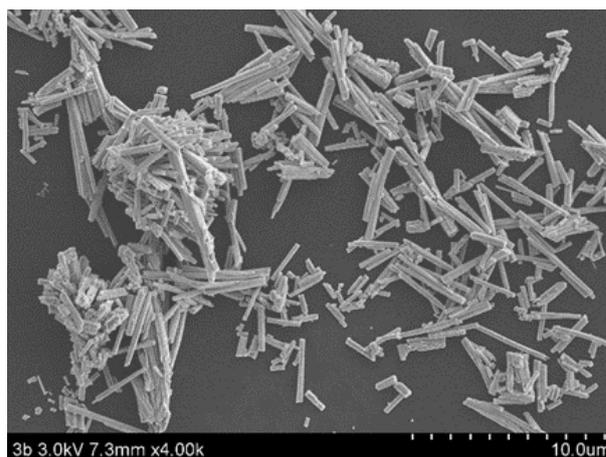


Figure 1: SEM image of catalyst (No. 3) before CO₂ hydrogenation process.

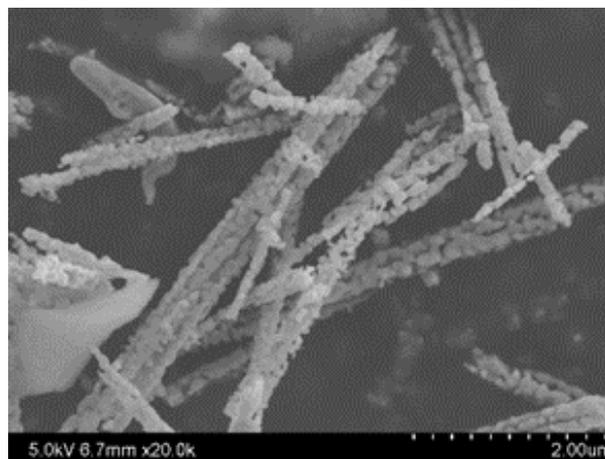


Figure 2: SEM image of catalyst (No. 3) after CO₂ hydrogenation process.

Functional Carbon-Dots as Effective and Sustainable Lubricant Additives

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Abstract

Carbon dots (CDs) are fluorescent nanoparticles exhibiting physical and optical properties somewhat comparable to those of semiconductor quantum dots (SQDs). However, CDs have exceptional hallmarks in comparison with heavy metal SCQDs: ease of synthesis from carbon-based materials, excellent biocompatibility, non-toxicity, low cost and chemical stability. All these their properties, along with the easy surface functionalization or passivation, make CDs ideal candidates for multiple applications in different areas. In recent years, much attention has been paid to the use of different kind of nanoparticles as lubricant additives [1,2]. In the case of carbon-based nanoparticles (graphene, carbon nanotubes or fullerenes), the dispersion stability in base oils is a problem waiting to be solved. The present work is focused on three aspects: a) the green-synthesis of CDs from glutathione and wasted tea leaves and grape husk, b) CDs surface functionalization to enhance their solubility in non-aqueous media and oils and c) use of such modified CDs as additives to lubricant oils in order to improve their tribological performance and increase the useful life of lubricating oils.

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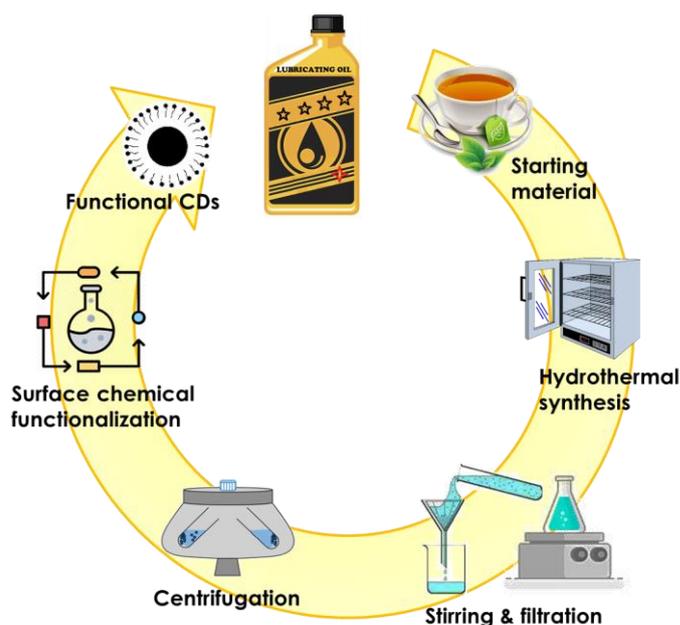


Figure 1: Graphic representation of CDs synthesis from wasted leaves of tea.

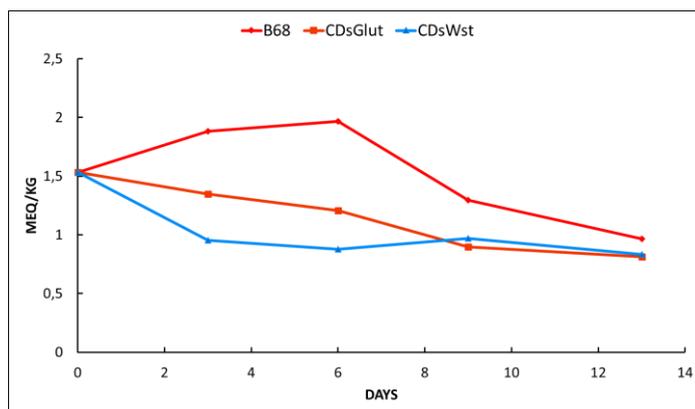


Figure 2: Effect of different functional CDs on the aging of Base oil (B68) quantified by the peroxides formation.

Monte Carlo Simulations for 2D Materials: Parallelization Strategy and Degeneracy in MoS₂

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Two-dimensional (2D) materials have stood out in the last years in the search for going beyond Silicon in electronic device applications. Graphene is the best example in this area, although 2D transition metal dichalcogenides are also very well positioned. There is a real need of fully examine the electronic transport in these novel materials using advanced physically based numerical models. Among them, ensemble Monte Carlo (MC) simulations offer great advantages due to their intrinsic relation to the nanoscale stochastic and quantum-mechanical transport processes. Our in-house ensemble MC simulator has been successfully employed in the study of graphene, silicene or transition metal dichalcogenides as molybdenum disulfide (MoS₂) [1, 2, 3]. In the present work, for the first time, we have focused on the analysis of the effects of degeneracy in MoS₂ using a MC tool taking into account Pauli exclusion principle and the renormalization of the electron-phonon coupling through the addition of the dielectric function [4, 5, 6, 7]. On the other hand, in order to expand the possibilities of our MC simulator and to lighten the large computational burden linked to these simulations, we have also developed a parallelization strategy of our code. The MC method for electron transport in semiconductors is based on several numerical and computational algorithms used to approximate complex mathematical expressions (related to the probabilities of scattering in solids, etc.) using repeated random sampling, even if

they are deterministic [8]. The parallelization is not a trivial task due to the fact that the motion of the set of particles, mimicking Boltzmann Transport Equation (with classical free flights interrupted by quantum-mechanical scatterings) depends on their prior motion and cannot be performed independently [9]. Besides, the parallelization of the developed sequential simulator makes the transition to a parallel MC simulator even more challenging.

The Message Passage Interface (MPI) is used to parallelize our MC simulator (written in Fortran programming language). In the first instance, the implemented physical model and the features of the simulator are needed to be analysed in depth.

Results for the impact of degeneracy in MoS₂ and the improvement of the CPU times in the simulation of 2D materials will be discussed.

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Acknowledgments

This work has been funded by research project TEC2016-80839-P financed by Ministerio de Economía y Competitividad (Spain) and FEDER (European Union), JCYL (Regional government) and European Social Fund via PhD Grant SA176-15, and the Project HPC-EUROPA3 (INFRAIA-2016-1-730897), with the support of the EC Research Innovation Action under the H2020 Programme.

Surface modification and characterization of conductive nanostructured PEDOT:PSS thin films

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Abstract

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) has emerged to be one of the most promising flexible electrode materials over rigid metallic oxides. This conducting polymer finds applications in many electric devices, such as OSCs, nanotransistors, supercapacitors, OLED, LCD, and wearable electronics [1]. In the past few years, many studies have been focused on the improvement and tuning of PEDOT:PSS electric and mechanical properties, by acting on its composition and/or surface structure [2]. In our present work, we investigated the formation of surface nanostructures on PEDOT:PSS thin film surfaces, after treatment with different low boiling point solvents. The thin films were obtained by spin coating polymer solutions on ITO substrates. Afterwards, the obtained samples were solvent treated by different methods, as spin coating a drop of pure solvent on top, solvent washing, and solvent vapour annealing. We studied the solvent treated PEDOT:PSS thin films by a combination of macroscopic and microscopic techniques. In particular, we evaluated the resulting structures by four-point probe, contact angle, and Atomic

Force Microscopy (AFM). AFM was used not only to evaluate the surface structures, but also to obtain mechanical and electrical properties. We observed that different PEDOT:PSS nanostructures were formed depending on the solvent nature and treatment procedure, with distinct physico-chemical properties. We discuss our results by considering the possible disposition of the PEDOT and PSS phases in the material before and after solvent treatment, since the nanostructured phase morphology will then affect significantly the polymeric layer characteristics [3,4].

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Optical Characterization of Nanoporous Alumina-based Structures Modified by ALD Technique

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Nanoporous alumina structures (NPASs) that were obtained by the two-step anodization method present highly organized porous structure with straight pores and small pore dispersion (Fig. 1a), high surface area and transmittance. Moreover, the possibility of easy surface material and pore radii modifications by a well-established technique such as atomic layer deposition (ALD) makes these nanoporous alumina-based structures (NPA-bSs) excellent platforms for different applications (chemical/biological sensors, drug delivery, nanofilters, photonic crystals,...) [1-4].

In this work, we study structural and optical changes for a NPAS associated to its coverage by a layer of different metal oxides (Al_2O_3 , SiO_2 , TiO_2 , Fe_2O_3 or ZnO) by ALD technique (Figure 1b) for NPA-bS samples with similar geometrical parameters (average pore radii ~ 9 nm and porosity ~ 7 %) according to SEM/TEM images analysis. Optical characterization was carried out by transmittance and spectroscopic ellipsometry measurements, while SEM, EDX and XPS analysis were performed for morphological and chemical surface changes, also using XPS depth-profile analysis for establishing the presence of coating material into the nanopore walls. Changes in samples characteristic optical parameters such as band-gap, refraction index and extinction coefficient depending on the cover layer material were determined. Moreover, the effect of samples geometry (pore size and porosity) on optical parameters was also considered.

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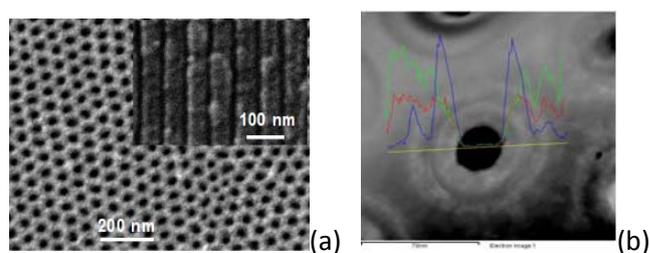


Figure 1: (a) SEM images of surface and cross-section of the NPAS. (b) TEM image of the ZnO covered sample (NPAS+ZnO): Al (green line), O (red line), Zn (blue line).

Magnetolipogels: a combined strategy for controlled drug release

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Supramolecular magnetogels comprise supramolecular hydrogels and magnetic nanocomposites, which allow the tailoring and modulation of the matrix structure and properties [1,2]. Here, the nanosystems stabilization remains a main challenge, as it has to ensure efficient drug encapsulation and avert the leaching out of nanoparticles. Hereby, in this work, lipid-coated nanoparticles incorporated in peptide hydrogels (magnetolipogels) were evaluated as a strategy for magnetogels development. Lipid-fibre interface domains averted leaching out of nanoparticles (figure 1). Further, the heating generation profiles were improved and triggered-release of doxorubicin was reproducible (figure 2). Overall, the here developed lipid-coated nanoparticles showed promising results for the development of supramolecular magnetolipogels aiming at the control of drug release.

References

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Figures

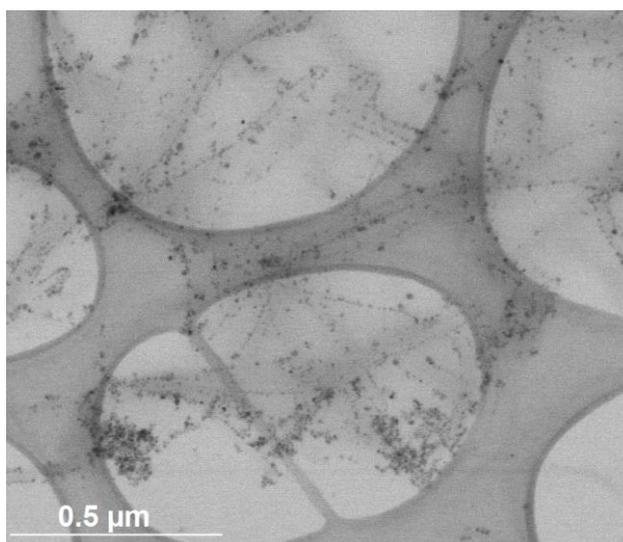


Figure 1: STEM image of the magnetolipogel (in a carbon honey-type mesh). Nanoparticles are adsorbed to fibres.

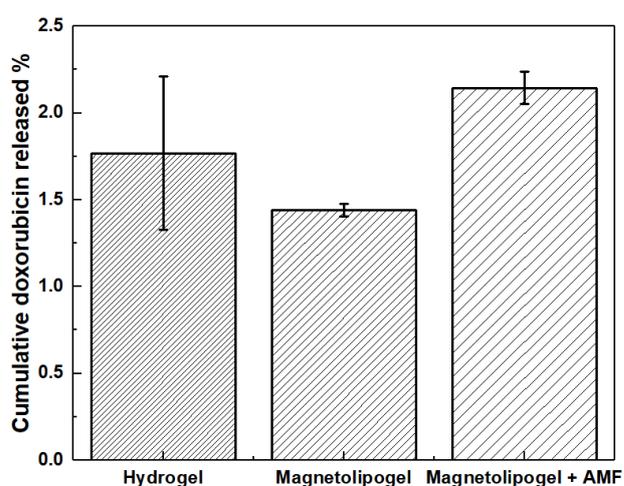


Figure 2: Comparison of cumulative doxorubicin released after 6 h from the hydrogel and magnetolipogel, with and without application of an alternating magnetic field for 30 min (AMF).

Synthesis of novel hybrid Au-TiO₂ nanoparticles for plasmonic photocatalysis in water remediation

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Abstract

Titanium dioxide (TiO₂) is one of the most used photocatalysts during wastewater treatment due to its relevant properties. However, TiO₂ is limited by its large bandgap (≈ 3 eV), which results in poor efficiency upon visible light irradiation.[1] To overcome this limitation, Au can be employed because its characteristic localised surface plasmon resonance band takes place in the visible region. Nevertheless, most of the works use the spherical gold nanoparticles in Au:TiO₂, [2] limiting the spectral irradiation region in the 500-550 nm, and wasting a large portion of visible radiation. Herein, new methods have been explored to synthesis hybrid Au:TiO₂ nanoparticles with metal shape anisotropy that expand the plasmonic absorption covering both visible and near IR regions.

References

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- [2] Kochuveedu ST, Jang YH, Kim DH, Chem. Soc. Rev., 42 (2013) 8467-8493

Figures

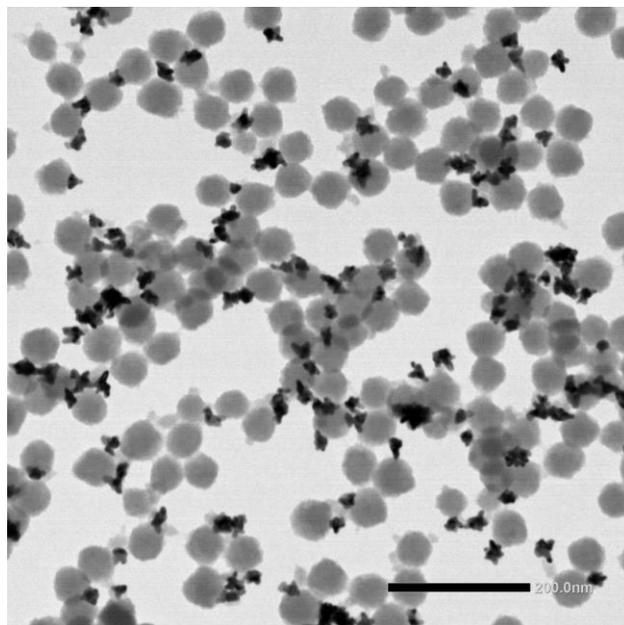


Figure 1: TEM image of hybrid Au:TiO₂ nanoparticles synthesized

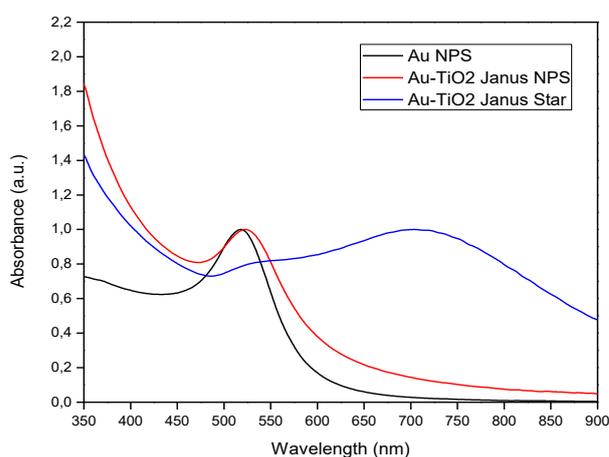


Figure 2: Absorption spectra of gold, hybrid Au:TiO₂ nanoparticles with different morphology by UV-Vis.

Microdisks: production and internalization by skin cancer cells

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Planar nano and micro disks made of magnetic materials are very promising in novel biomedical applications.[1] Particles with large magnetic moments and non-spherical shapes provide outstanding properties for cell manipulation, biosensing, and magneto-mechanical actuation. Fabrication of these geometries requires top-down lithography processes and usually a low production yield.[2] This work reports on the optimization of the process at each stage, from the patterning to the detachment of disks and the sterilization of the solution. Figure 1 presents a scanning electron image (SEM) at the end of the process, a drop of dispersed microdisks in water dried on a silicon wafer. It is worth noting that these large microdisks are still in a magnetic vortex state, and therefore, they are suitable for biotechnological applications. The viability of the microdisks for cellular studies was tested in-vitro assays. Cytotoxicity and internalization of the particles were investigated for periods of 24 hours. Figure 2 shows an optical image of microdisks internalized by macrophages

RAW 264.7 and MeWO tumoral cells. Work supported by MINECO FIS2016-76058 (AEI/FEDER, UE), EU grant H2020-MSCA-734801, GV IT1162-19 and PIBA 2018-11.

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Figures

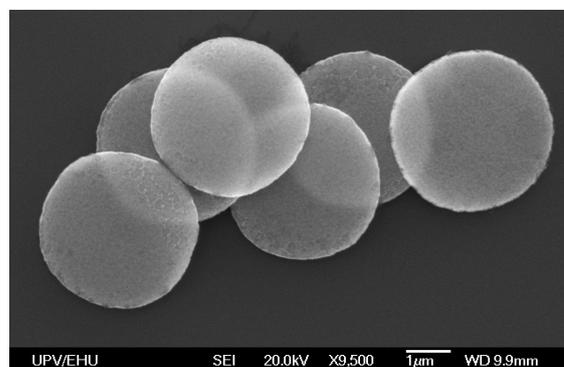


Figure 1: SEM image of detached magnetic microdisks dried on a Si wafer.

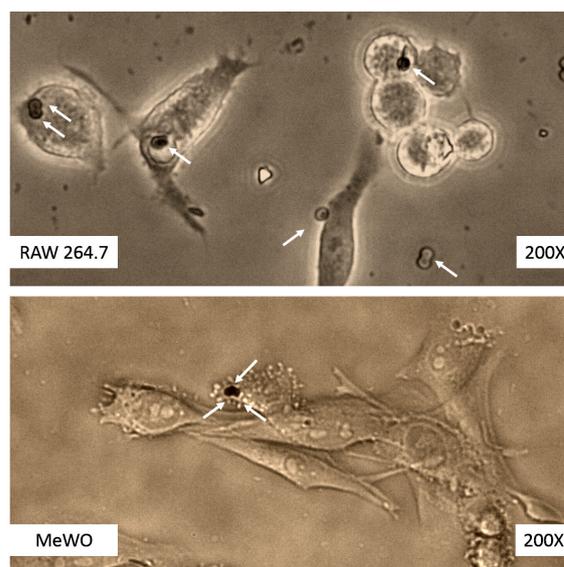


Figure 2: Optical image of macrophages (RAW 264.7) and skin cancer cells (MeWOskin) with internalized magnetic microdisks.



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