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TNT 2019
Trends in NanoTechnology

ABSTRACTS BOOK

TNT2019 Foreword

On behalf of the International and Technical Committees, we take great pleasure in welcoming you to San Sebastian (Spain) for the "Trends in NanoTechnology" International Conference (TNT2019).

TNTconf series is celebrating its 20th anniversary with a high-level scientific program addressing key factors for the future of the Nanoscience and Nanotechnology community in Europe.

TNT2019 is being held in large part due to the success of earlier TNT Nanotechnology Conferences. TNT events have demonstrated over the past 20 years that they are particularly effective in transmitting information and promoting interaction and new contacts among workers in this field. Furthermore, this event offers visitors, exhibitors and sponsors an ideal opportunity to interact with each other.

This year, a "Graphene and 2DM" one-day Symposium will again be organized within TNT2019 in collaboration with ICN2 (Spain).

We are indebted to the following Scientific Institutions, Companies and Government Agencies for their financial support: Phantoms Foundation, Consejo Superior de Investigaciones Científicas (CSIC), Donostia International Physics Center (DIPC), ACS Nano and Royal Society of Chemistry (RSC).

We would also like to thank the following entities for their participation: Hiden Analytical.

In addition, thanks must be given to the staff of all the organizing institutions whose hard work has helped planning this conference.

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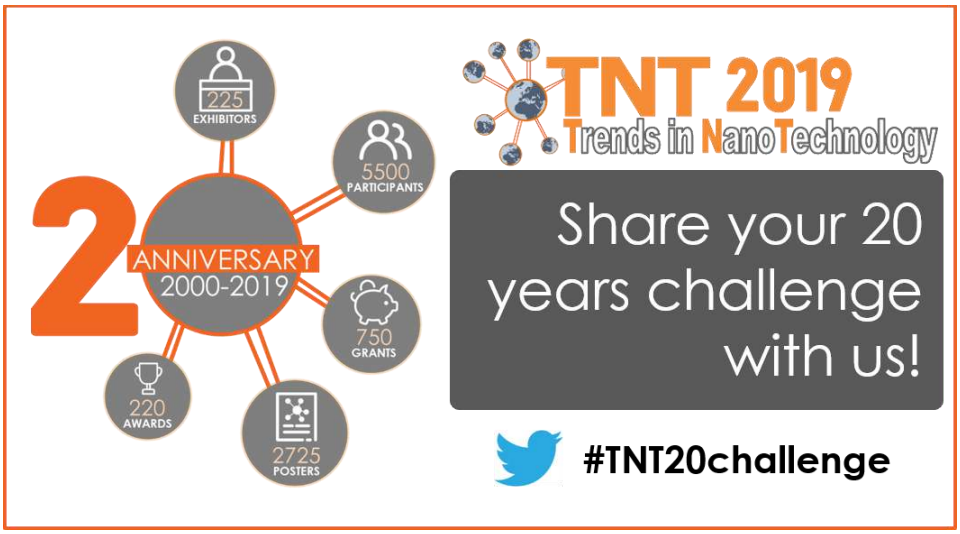

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TNT2019 Speakers

KEYNOTES
contributions

Atomic-scale interactions in plasmon-enhanced molecular spectroscopy

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Surface-enhanced molecular spectroscopy relies on the effect of enhanced electromagnetic fields to boost the signal from electronic and vibrational molecular excitations. Through the years, techniques such as fluorescence, infrared absorption, or Raman scattering have taken advantage of plasmonic nanoantennas to achieve such a signal enhancing effect. As fabrication and chemical synthetic methods are standardly reaching atomic-scale configurations, for instance in plasmonic nanogaps, more sophisticated theoretical methods are needed to address the quantum nature of electronic states, or to account for the quantization of plasmonic fields. Here, we report the effect of strongly inhomogeneous fields, localized at the atomic scale, as in tunneling gaps or in nanoparticle-on-a-mirror (NPoM) configurations, to modify fluorescence in molecules, as well as selection rules in plasmon-enhanced Raman scattering [1]. The presence of "picocavities" in plasmonic gaps redefines the landscape of Raman molecular activit. By adopting *ab-initio* methods to obtain the electronic structure and vibrational fingerprints of organic molecules, the effect of these field inhomogeneities can be properly considered, providing an understanding of relevant spectral information, including strong coupling of molecular emitters, and molecular optomechanics. On the other hand, the quantization of plasmonic fields, following cavity-Quantum Electrodynamics (QED) methods [2], can be also considered to reveal the complex dynamics of molecular fluorescence from hybrid molecule-cavity polaritonic branches, or to trace the population of vibrations interacting with a plasmonic cavity, pumped by a detuned external laser field. Strong non-linear effects and correlations in the emission can be identified in both types of photon emission thanks to the quantum nanooptics framework [3]. The quantum regime in surface-enhanced molecular spectroscopy is currently at hand, and accurate quantum theories can reveal a new variety of phenomena with implications in the control of quantum molecular states, as well as in plasmon-induced chemical reactivity.

References

[1] T. Neuman, R. Esteban, D. Casanova, F. J. García-Vidal, and J. Aizpurua, Nano Lett. **18**, 2358-2367 (2018)
[2] M.K. Schmidt, R. Esteban, A. González-Tudela, G.Giedke, and J. Aizpurua, ACS Nano **10**, 6291-6298 (2016)
[3] F. Benz, M. K. Schmidt, A. Dreismann, *et al*. Science **354**, 726-729 (2016) .

Figures

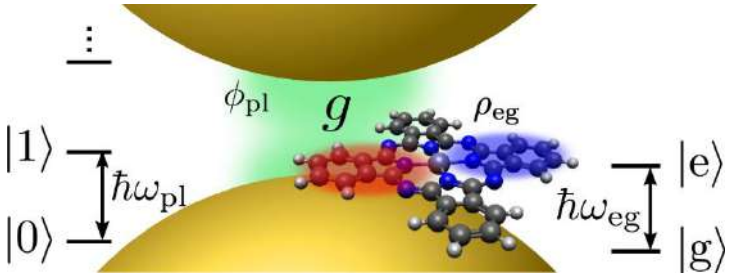

Figure 1. Schematic representation of a plasmonic cavity where an optical resonance at energy $\hbar\omega_{\rm pl}$ produces an electromagnetic potential $\phi_{\rm pl}$, which interacts at a coupling rate g, with an excitonic state of a molecule with energy $\hbar\omega_{\rm eg}$, characterized by an electronic transition density $\rho_{\rm eg}$.

Quantum transport in nanopatterned graphene - without killing the patient

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After the initial excitement about graphene's high performant and scientifically rich electronic properties, one of the most obnoxious roadblocks have been to pattern graphene on a small scale. In theory, nanostructuring of graphene opens for the electronic and photonic properties to be "programmed" to match specific applications or to bring out entirely new physics. In practice, even low levels of edge disorder and contamination associated with even the best lithographic processes, ruins the electronic properties. This has effectively shut down the hope of controlling transport at the quantum level, as well as trivially downscaling graphene electronic components to scales common for mainstream silicon electronics. I will discuss progress we have made in engineering the graphene edges[1,2], and focus on a recent example [3]. We show that by combining encapsulation in hexagonal boron nitride with high-density lithography, and carefully tuning the etching process, we are able to pattern graphene on the 10 nm scale (Fig. 1), and still preserve the detailed magnetotransport signatures predicted by tight-binding calculations. The surprising survival of the subtle moire-superlattice signatures associated with twisting of the crystalline interlayers opens for construction of circuits and components that exploit this emerging branch of solid-state physics.

References

[1] J. M. Caridad, G Calogero, P Pedrinazzi, J E Santos, A Impellizzeri, T Gunst, T J Booth, R Sordan, P Bøggild, M Brandbyge, A graphene-edge ferroelectric molecular switch, **Nano Letters**, 18, 8, 4675-4683 (2018)
[2] J. M. Caridad, S. R. Power, M. R. Lotz, A. Shylau, J. D. Thomsen, L. Gammelgaard, T. J. Booth, A-P Jauho, P. Bøggild, Conductance quantization suppression in the quantum Hall regime, **Nat. Comm.** , 9:659 (2018)
[3] B. S. Jessen, L. Gammelgaard, M. R. Thomsen, D. M. A. Mackenzie, J. D. Thomsen, J. M. Caridad, E. Duegaard, K. Watanabe, T. Taniguchi, T. J. Booth, T. G. Pedersen, A-P. Jauho, P. Bøggild, **Nature Nanotech.**, 2019, 10.1038/s41565-019-0376-3

Figures

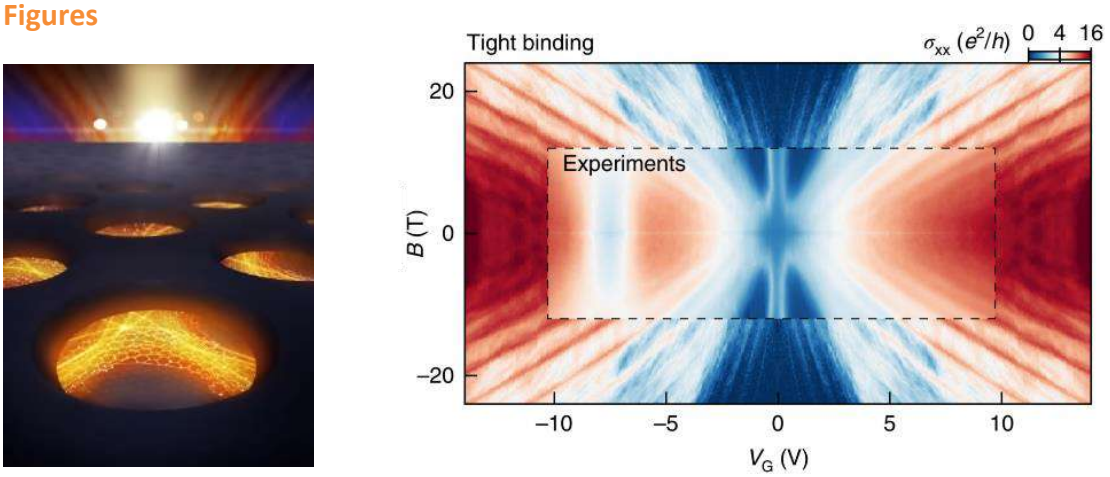

Figure 1. By carefully etching holes in graphene through a protective encapsulation layer of hexagonal boron nitride (left), with a spacing of just 12 nanometers, the electronic band structure can be engineered in a deterministic way (right).

Optical Hall effect and Veselago lensing in graphene

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When passing an optical medium in the presence of a magnetic field, the polarization of light can be rotated either when reflected at the surface (Kerr effect) or when transmitted through the material (Faraday rotation). This phenomenon is known as a direct consequence of the optical Hall effect arising from the light-charge carrier interaction in solid state systems subjected to an external magnetic field, in analogy with the conventional Hall effect. The optical Hall effect has been explored in many thin films and also more recently in 2D materials. An alternative approach based on strain engineering is proposed here to achieve an optical Hall conductivity in graphene without magnetic field [1]. Indeed, strain induces lattice symmetry breaking and hence can result in a finite optical Hall conductivity as predicted by first-principles and tight-binding calculations.

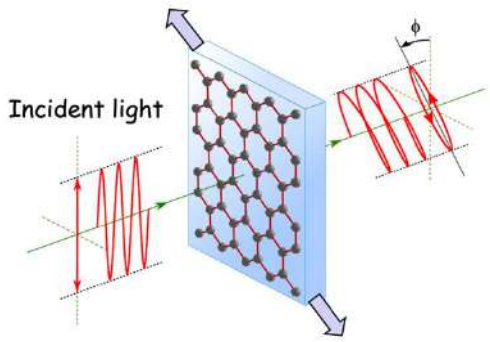
At p-n boundaries, graphene Dirac fermions behave as would photons encountering a negative index media, therefore experiencing a peculiar refraction known as Veselago lensing. However, the way Dirac fermions flow through a Veselago lens remains largely unexplored. Here, a novel approach to create a movable and highly tunable circular Veselago lens in graphene is proposed, based on the polarized tip of a scanning gate microscope and tight-binding simulations [2]. In particular, a high current density in the lens core, as well as two low current density points along transport axis, are evidenced, strongly depending on the p-n junction smoothness [2]. This research paves the way towards a deep understanding of Dirac fermions to engineer relativistic electron optical devices.

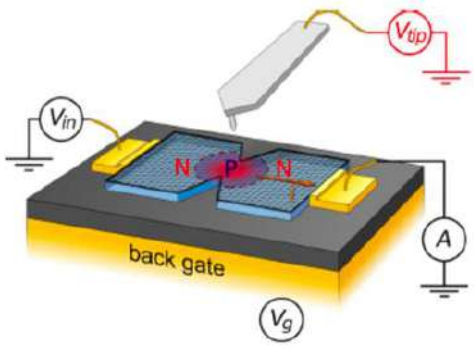
References

[1] *Optical Hall effect in strained Graphene*
V.-H. Nguyen, A. Lherbier, and J.-C. Charlier, 2D Materials **4**, 025041 (2017).

[2] *Imaging Dirac fermions flow through a circular Veselago lens*
B. Brun, N. Moreau, V.-H. Nguyen, J.-C. Charlier, C. Stampfer, and B. Hackens,
Phys. Rev. B **100**, 041401(R) (2019).

Figures





Recent Advances in Physics and Materials Science of Magnetic Topological Insulators

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Topological insulators (TIs) are narrow–gap semiconductors characterized by the gapless Dirac-like surface state and protected by time-reversal (TR) symmetry. Two-dimensional TIs or quantum spin Hall insulators (QSHIs) are realized in thin film insulators and possess this state at the film edge where spin transport can be effectuated. Introduction of a magnetic field (external or internal) breaks TR symmetry and causes splitting of the topological surface state at the Dirac point thus making the surface insulating. These ferromagnetic TIs realize quantum anomalous Hall effect (QAHE) in two-dimensional systems. Internal magnetic field in TIs can be created in various ways, in particular, by introducing vacancies or carbon atoms [1], doping with 3d-transition metal atoms [2], displaying magnetic semiconductors or organic overlayers as well as bulk materials on the surface of three- or two-dimensional TIs [3-5]. Magnetic field effect on the TI surface state (SS) can be also realized due to extension of the TI SS into the magnetic overlayer [6-9]. Antiferromagnetic TIs can realize such intriguing effects as magnetoelectric effect [10] and axion insulator phase [11]. Here I present and discuss recent results of the study of nonmagnetic, ferro-, and antiferro-magnetic topological insulators and heterostructures.
New method for engineering of heterostructures that results systematically in a big splitting of the Dirac cone [6-9,12] is discussed and new perspectives for realizations of exotic topological phases are outlined.

References

[1] S. Roy et al., Phys. Rev. Lett. 113 (2014) 116802.
[2] J. Henk et al., Phys. Rev. Lett. 109 (2012) 076801.
[3] V.N. Men'shov et al. Phys. Rev. B 88 (2013) 224401.
[4] M.M. Otrokov, E.V. Chulkov, and A.Arnau, (2015), Phys. Rev. B 92 (2015) 165309.
[5] S.V. Eremeev et al., (2013), Phys. Rev. B 88 (2013) 144430.
[6] T. Hirahara et al., Nano Letters, 17, 3493 (2017).
[7] M.M. Otrokov et al., JETP Lett. 105, 297 (2017).
[8] M.M.Otrokov et al., 2D Materials, 4, 025082 (2017).
[9] S.V.Eremeev, M.M.Otrokov, and E.V.Chulkov, Nano Letters, 18, 6521 (2018).
[10] R.S.K.Mong, A.M.Essin, and J.E.Moore, Phys. Rev. B 81 (2010) 245209.
[11] J.Wang, B.Lian, and S.-C.Zhang, Phys. Rev. B 93 (2016) 045115.
[12] M.M.Otrokov et al., Phys. Rev. Lett. 122, 107202 (2019).

Novel magnetic proximity effect in vertical structures of 2D ferromagnets and graphene

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Magnetic proximity effect is very often portrayed as a spin splitting induced in the energy levels of a non-magnetic material because of its exchange interaction with an underlying magnetic material. The resulting spin splitting might lead to spin-dependent properties in the non-magnetic material. In this talk I will discuss a new class of magnetic proximity [1] effect that is based on a spin dependent hybridization of the electronic states at the Fermi energy of a non-magnetic conductor with a flat spin-polarized band of a ferromagnetic insulator. In the case of a conducting non-magnetic 2D crystal, spin dependent hybridization with a ferromagnetic insulator can opens up a gap in one spin channel only, resulting in a half-metal. I will illustrate this effect in the case of Dirac electrons in monolayer graphene with the spin-polarized flat conduction band of a monolayer CrI_3 [2]. I will show that an off-plane electric field controls the hybridization and I will discuss a very efficient spin valve based on hybridization proximity.

References

[1] C. Cardoso, J. Fernández-Rossier, Hybridization magnetic proximity effect, in preparation
[2] C. Cardoso, D. Soriano, N. A. García-Martínez, J. Fernández- Rossier**,** Van der Waals spin valves, Physical Review Letters **121**, 067701 (2018)

Metal oxide materials as a sustainable alternative to low cost and flexible electronics

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Metal oxide semiconductors are a good example as a success story in the area of thin film electronics, since it took less than 10 years after the discovery until the commercialization of the first products mainly in the area of displays. The main advantages of these materials are the low temperature processability, the high mobility and the uniformity over large areas, since they present an amorphous structure.
Nevertheless to decrease costs associated to electronic devices a strategy is using cheap and abundant materials in conjunction with low cost fabrication methods, associated to an overall increase of electrical performance. This is why metal oxide semiconductors are the key materials since they are chemically stable, mostly non-toxic and abundant materials, often manufactured by low cost methods, under ambient conditions. Consequently, devices made of metal oxides are inexpensive, very stable and environmentally safe, the 3 most important requirements for electronics.
Despite being explored for more than a century for electronic applications, from the initial works of Badeker in 1907 with CdO to the cutting edge IGZO available these days in active matrix backplanes of flat panel displays, oxides still present an exceptional and innovative combination of properties not achievable by any other material class. In fact, they are true multifunctional materials, being able to exhibit optical transparency, conducting / semiconducting / insulating behaviour, piezoelectricity and catalytic or self-cleaning properties among many others.
In this presentation we will review some of the most promising new technologies based on oxide conductors, semiconductors, dielectrics as well as electrochromic devices either in the form of nano-films or nanoparticles, and we will summarize the major milestones already achieved with this emerging and very promising technology focused on the work developed in our laboratory.
By using these materials and technologies we are contributing to the evolution of environmentally conscious electronics that is able to add new electronic functionalities onto surfaces, which currently are not used in this manner.

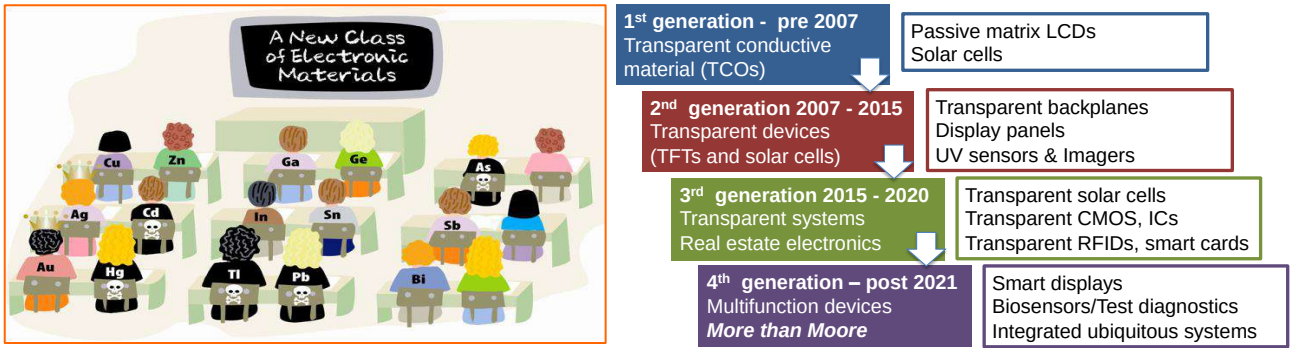

Figure 1. A comparison between a classroom and the new class of electronic materials based on metal oxides, by Prof. J. Wager from Oregon State University and the evolution of metal oxide materials.

References

[1] E. Fortunato, P. Barquinha, and R. Martins, "Oxide Semiconductor Thin-Film Transistors: A Review of Recent Advances," Advanced Materials, vol. 24, pp. 2945-2986, Jun 12 2012.

[2] P. Barquinha, R. Martins, L. Pereira and E. Fortunato, Transparent Oxide Electronics: From Materials to Devices. West Sussex: Wiley & Sons (March 2012). ISBN 9780470683736.

Control of Light at the Atomic Scale

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Plasmons in atomic-scale structures exhibit intrinsic quantum phenomena related to both the finite confinement that they undergo and the small number of electrons on which they are supported. Their interaction with two-level emitters is also evidencing strong quantum effects. In this talk we will discuss several salient features of plasmons in atomic-scale materials, such as graphene and atomic layers of noble metals. In particular, we will explore their ability to mediate ultrafast heat transfer [1], the generation of high harmonics [2], their interaction with molecules and quantum emitters [3], and their extreme nonlinearity down to the single-photon level [4]. We will further analyze intriguing details in the plasmonic response of atomically-thin crystalline films of silver, the plasmons of which have been recently revealed experimentally [5].

References

[1] R. Yu, A. Manjavacas, and F. J. García de Abajo, Nat. Commun. **8**, 2 (2017).
[2] J. D. Cox and F. J. García de Abajo, Acc. Chem. Res. DOI: 10.1021/acs.accounts.9b00308
[3] E. J. C. Dias and F. J. García de Abajo, ACS Nano **13**, 5184 (2019)
[4] J. D. Cox and F. J. García de Abajo, Nano Lett. **19**, 3743 (2019)
[5] Z. M. Abd El-Fattah et al., ACS Nano **13**, 7771 (2019)

Sensing Performance of Hybrid Magnetoplasmonic Systems

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Plasmonic structures are widely used in low-cost, label-free biosensors, and the investigation of how to improve their sensitivity or to widen their range of applications is a central topic in the field of plasmonics.[1,2] The most commonly used plasmonic sensors are based on the concept of surface plasmon resonance (SPR) and, in particular, on the sensitivity of these resonances to changes in the refractive index of the medium surrounding a metallic structure.

In the search for an improved bulk sensitivity of SPR-based sensors, researchers have proposed different strategies. Thus, for instance, it has been shown that the use of the magneto-optical properties of layered systems containing magnetic materials can, in principle, enhance the sensitivity of these sensors.[3,4] Another possibility that is becoming increasingly popular is the use of nanohole arrays or perforated metallic membranes featuring arrays of subwavelength holes. [5,6] These sensors make use of the extraordinary optical transmission phenomenon, which originates from the resonant excitation of surface plasmons in these periodically patterned nanostructures.

We present two case studies showing how the use of hybrid magnetoplasmonic systems comprising in one case 2D crystals using ferromagnetic and noble metals and in the other bare noble metal nanoparticles, lead to a notable enhancement of the sensing performance plasmonic sensors. In particular, we present perforated Au−Co−Au films with a periodic array of subwavelength holes as transducers in magneto-optical surface-plasmon-resonance sensors and a random collection of Au nanoparticles supporting localized plasmon resonances deposited over a glass substrate, but using as transducer signal the measurements of the transverse magnetooptical Kerr effect (TMOKE). We demonstrate that this detection scheme results in (i) bulk figures of merit that are two orders of magnitude larger than those of any other type of plasmonic sensor [7], and an increase of ca. 300% in the refractive index sensing lowering at the same time the limit of detection in a ca. 200% [8]. The sensing strategy put forward here can make use of the different advantages of nanohole-based plasmonic sensors such as miniaturization, multiplexing, and its combination with microfluidics.

References

[1] O. Tokel, F. Inci, U. Demirci, Chem. Rev. **114**, (2014) 5728
[2] M.-C. Estevez, M. A. Otte, B. Sepulveda, L. M. Lechuga, Anal. Chim. Acta **806**, (2014) 55
[3] B. Sepúlveda, A. Calle, L.M. Lechuga, G. Armelles, Opt. Lett. **31**, (2006) 1085
[4] M.G. Manera, *et al.*, Biosens. Bioelectron. **58**, (2014) 114
[5] A.A. Yanik, *et al.*, Proc. Natl. Acad. Sci. U. S. A. **108**, (2011) 11784
[6] A.E. Cetin, *et al.*, ACS Photonics **2**, (2015) 1167
[7] B. Caballero, A. García-Martín, and J. C. Cuevas, ACS Photonics **3**, (2016) 203
[8] M.G. Manera, *et al.,* Scientific Reports **8**, (2018) 12640

Wigner crystals in transition-metal dichalcogenides: optical detection and quantum simulation

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Cold atoms in optical lattices and trapped ions have proved to be an exciting and fruitful playground to explore quantum many-body physics and serve as quantum registers.

We explore the possibility to realize an analogous regular and tunable array of charge carriers in semiconductor structures. Wigner crystals in transition-metal dichalcogenides prove to be a promising platform to realize such structures.

We characterize the requirements for the Wigner crystallization in this setting and for the appearance of quantum effects in the ground state of the system. We analyze which spin systems can be simulated in this setting and we propose optical methods for the read-out and manipulation of the quantum spin system.

Plasmon-assisted photoregeneration of biomolecules.

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Spurred by outstanding optical properties, metallic nanoparticles have attracted much attention in the photocatalysis-based research community. The interaction of metallic nanoparticles with light invokes localized surface plasmon resonance that through fast decay enhances near optical field, generates hot carriers, or rises local temperature, increasing the overall rate of a given chemical reaction.
We present here the use of gold nanoparticles with multiple shapes and surface functionalizations (Pd, Pt) towards the photoregeneration of nicotinamide adenine dinucleotide, an essential biomolecule participating in light processes of natural photosynthesis [1-3]. The nanoparticle-based catalysts were either assembled in the form a plasmonic film on a glass substrate or combined with hydrogel microbeads as well as cellulose fibers, allowing thus their facile handling without altering optical properties. We found out that photocatalytic activities depend not only on the degree of the shape anisotropy but also on the spatial distribution of co-catalyst on the photocatalyst surface. We will also resolve the mechanism of cofactor reduction in the presence of state-of-the-art electron donor molecules – triethanolamine - showing that its degradation products can alter energy flow, leading to a scenario unrelated to the photocatalytic mechanism in question but to the process driven by unexpectedly formed intermediates [4].

References

[1] Sánchez-Iglesias, A.; Chuvilin, A.; Grzelczak, M. Plasmon-Driven Photoregeneration of Cofactor Molecules. *Chem. Commun.* **2015**, 51, 5330

[2] Sánchez-Iglesias, A.; Barroso, J.; Martinez-Solis, D.; Taboada, J. M.; Obelleiro-Basteiro, F.; Pavlov, V.; Chuvilin, A.; Grzelczak, M. Plasmonic Substrates Comprising Gold Nanostars Efficiently Regenerate Cofactor Molecules. *J. Mater. Chem. A* **2016**, 4, 7045

[3] Kinastowska, K.; Barroso, J.; Yate, L.; Pavlov, V.; Chuvilin, A.; Bartkowiak, W.; Grzelczak, M. Cobalt Oxide as a Selective Co-Catalyst for Water Oxidation in the Presence of an Organic Dye. *Photochem. Photobiol. Sci.* **2017**, 16, 1771

[4] Kinastowska, K.; Liu, J.; Tobin, J. M.; Rakovich, Y.; Vilela, F.; Xu, Z.; Bartkowiak, W.; Grzelczak, M. Photocatalytic Cofactor Regeneration Involving Triethanolamine Revisited: The Critical Role of Glycolaldehyde. *Appl. Catal. B: Environmental* **2019**, 243, 686

Crystal Growth in the Flatland: Growth Mechanisms in 2D Materials and Pathways to Scalable, Controlled Device Integration

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In order to serve the industrial demand for "electronic-grade" 2D materials, we focus on developing chemical vapour deposition (CVD) processes, and in this talk I will review our recent progress in scalable CVD [1] and device integration approaches of highly crystalline graphene, hexagonal boron nitride (h-BN) and transition metal dichalcogenide films (using MOCVD of WS_2 as example). The systematic use of in-situ metrology, ranging from high-pressure XPS to environmental electron microscopy, allows us to reveal some of the key growth mechanisms for these 2D materials that dictate crystal phase, micro-structure, defects, and heterogeneous integration control at industrially relevant conditions.
h-BN not only is increasingly employed as support, encapsulant and barrier for 2D material technologies, but attracted recent interest as active material particularly for defect-induced sub-bandgap single photon emission at room temperature. We developed tailored CVD processes to achieve large monolayer h-BN domains with lateral sizes exceeding 1mm, coupled to application specific transfer methods [2]. We explore super-resolution imaging as means to h-BN layer characterization [3,4], and investigated approaches to control emitter stability/behavior and density/location for potential quantum applications. We also studied the role of less straightforward growth parameters such as dissolved species in the catalyst bulk, and here will highlight the significant effects of residual bulk oxygen in graphene and h-BN growth [5]. We show that such CVD graphene can sustain mobilities of 70000 cm2/Vs at RT even when initially wet-transferred [6]. We introduce the concept of solid catalysts for epitaxial growth of a semiconductor onto a 2D substrate, using the example of Ge growth on graphene or h-BN with an Au catalyst [7]. Free-standing graphene and h-BN membranes allow us to study such forms of epitaxy directly by ETEM. With ETEM we recently also discovered how a 2D layer forms on a liquid alloy droplet, and we discuss strategies to control the presence of such 2D surface phases, using it as a tool in designing strategies for nanostructure growth.

References

1. Hofmann et al., J. Phys. Chem. Lett. 6, 2714 (2015).
2. Wang et al., ACS Nano 13, 2114 (2019); Babenko et al. submitted (2019)
3. Stern et al., ACS Nano 13, 4538 (2019).
4. Comtet et al., Nano Lett. 19, 2516 (2019).
5. Burton et al., J. Phys. Chem. C 123, 16257 (2019).
6. De Fazio et al., ACS Nano (2019) doi.org/10.1021/acsnano.9b02621
7. Periwal, Ross et al, submitted (2019).
8. Panciera et al., Adv. Mater. 31, 1806544 (2019).

Novel Topological Phases in Ferroelectric Materials

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Complex topological configurations are a fertile area to explore novel emergent phenomena and exotic phases in Condensed-Matter Physics. The discovery of magnetic skyrmions one decade ago [1] have triggered a flurry of research on these particle-like nanometer-sized topologically protected spin textures, mostly motivated by their potential use in spintronic devices such as race track memories [2]. Since then, researchers have long wondered whether ferroelectrics may present topological textures akin to magnetic skyrmions and chiral bubbles. In this quest, the side by side advances in experimental growth and characterization techniques, and the development of new modelling tools are of paramount importance. In this respect, the emerging field of second-principles simulations [3-4], where an effective model is constructed by a judicious choice of the essential physics, and the parameters of the model are extracted by fitting to Density Functional Theory, are proving increasingly valuable in the study of large systems, overlapping in size with those that can be currently grown by atomic layer deposition methods. As a result of this continuous feedback between theory and experiment, the recent discovery of polarization vortices [5] and their associated complex-phase coexistence and response under applied fields in superlattices of $(PbTiO_3)_n/(SrTiO_3)_n$ [6] suggests the presence of a complex, multi-dimensional system capable of emergent physical responses, such as a chirality [7]. In this talk, I shall describe the latest developments to create, tune, and characterize topological textures in ferroelectrics [8,9]. Polar structures with a well-defined topological charge and chirality will be presented. The stabilization of such non-uniform polarization topology results in highly enhanced susceptibilities, and also provides a pathway for engineering novel functionalities previously inaccessible, such as regions with negative capacitance [10].

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References

[1] N. Nagaosa and Y. Tokura, *Nature Nanotechnology*, 8, 899-911 (2013), and references therein.
[2] S.S. Parkin, M. Hayashi, and L. Thomas, *Science*, 320, 190-194 (2008)
[3] J. Wojdel et al., *J. Phys.: Condens. Matter*, 25, 305401 (2013)
[4] P. García-Fernández et al., *Physical Review B*, 93, 195137 (2016)
[5] A.K. Yadav et al., *Nature*, 530, 198-201 (2016)
[6] A.R. Damodaran et al., *Nature Materials*, 16, 1003-1009 (2017)
[7] P. Shafer et al., *Proceedings of the National Academy of Sciences of the United States of America*, 115, 915-920 (2018)
[8] M. A. Pereira Gonçalves et al., *Science Advances*, 5, eaau7023 (2019)
[9] S. Das et al., *Nature* 568, 368 (2019)
[10] A.K. Yadav et al., *Nature,* 565, 468-471 (2019)

Two-probe scanning tunneling spectroscopy as a tool for studing quantum transport at the atomic-level

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Techniques based on multiprobe scanning tunneling microscopy (MP-STM) allow determination of charge and spin transport in variety of systems supported on surfaces of solid materials. In classical 2- and 4-probe methods STM tips are navigated by scanning electron microscope or high-resolution optical microscope typically in micrometer scales down to hundreds of nanometers. These MP-STM methods are currently regarded as universal tools for in-situ characterization of mesoscopic transport phenomena [1,2].

Such a mesoscopic experimental paradigm has recently been changed by downscaling of 2-probe STM experiments towards the atomic level [3,4]. In this case current source and drain probes are positioned in atomically defined locations with respect to the characterized nanosystems. These experiments rely on fully STM-based tip positioning protocol with probe-to-probe separation distances reaching tens of nm [3,4]. Such probe-to-probe lateral positioning precision is combined with pm vertical sensitivity in establishing probe-to-system contacts. These two factors enable realization of two-probe scanning tunneling spectroscopy (2P-STS) experiments, where transport properties can be characterized by macroscopic probes kept in well-defined tunneling conditions [4].

Here, on chosen examples, I will present application of 2P-STS methodology. First, I will show that 2P-STS can give information about quasi-ballistic (coherent) transport through one-dimensional π^* states of germanium dimer row wires [4]. Then, I will discuss 2P-STS methodology to probe quantum transport properties in a functional system: graphene nanoribbons (GNRs) epitaxially grown on the sidewalls of silicon carbide (SiC) mesa structures. These GNRs display ballistic transport channels with exceptionally long mean free paths and spin-polarized transport properties as proven by mesoscopic multiprobe transport experiments [5-7]. Interestingly, the nature of the ballistic channels remains an open question. I will show that 2P-STS experiments can give a new insight into quantum origin of these transport properties. Finally, I will discuss perspectives for broader application of multiprobe STM/STS.

References

[1] Li, A.-P. et al., Adv. Funct. Mater., 23 (20), 2509-2524 (2013)
[2] Voigtländer B. et al., Rev. Sci. Instrum., 89(10), 101101 (2018)
[3] Kolmer M. et al., J. Phys.: Condens. Matter, 29(44), 444004 (2017)
[4] Kolmer M. et al., Nat.Commun., 10, 1573 (2019)
[5] Baringhaus J., Nature, 506, 349–354 (2014)
[6] Aprojanz J. et al., Nat.Commun., 9, 4426 (2018)
[7] Miettinen A.L. et al., Phys. Rev. B 100, 045425 (2019)

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Light interaction with nanoresonators: mode volume and quasinormal mode expansion

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Microcavities and nanoresonators are characterized by their modes, called quasinormal modes because of they are the eigensolution of non-Hermitian operators. In contrast to waveguide and free space modes, quasinormal modes are not well documented in the literature, although nanoresonances play an essential role in current developments in nanophotonics. The reason is due to mathematical difficulties, see details in the recent review article [1], and especially to the fact that quasinormal modes cannot be normalized by their energy.

Quasinormal modes are characterized their quality factors Q and mode volumes V. While Q can be unambiguously defined and interpreted [1], there are still questions on V and in particular on its complex-valued character, whose imaginary part is linked to the non-Hermitian nature of open systems.

Mode Volume. The concept of complex V's [Phys. Rev. Lett 110, 237401 (2013)] is recent. It seems to be rooted in important phenomena of light-matter interactions in non-Hermitian open systems [1]. For instance, the ratio Im(V)/Re(V) quantifies the spectral asymmetry of the mode contribution to the modification of the spontaneous emission rate of an emitter weakly coupled to a cavity. For strong coupling, it modifies the usual expression of the Rabi frequency by blurring and moving the boundary between the weak and strong coupling regimes. Despite these strong roots, complex V are often seen as a mathematical abstraction.

Helped by cavity perturbation theory, see related earlier work in [2], and near field experimental data, we clarify the physics captured by the imaginary part of V and show how a mapping of the spatial distribution of both the real and imaginary parts can be directly inferred from perturbation measurements. This result shows that the mathematically abstract complex mode volume in fact is directly observable.

Quasinormal mode expansion. The modal theory of optical resonators has recently achieved very important improvements, to such an extend that we may say future works we mostly on refinements rather than on fundamental developments. At the conference, we will show state of the art reconstruction of the field scattered by resonators in their quasinormal mode basis [4].

References

[1] P. Lalanne, W. Yan, K. Vynck, C. Sauvan, and J.-P. Hugonin, Laser Photonics Rev. 12, 1700113 (2018). "Light interaction with photonic and plasmonic resonances"

[2] J. Yang, H. Giessen, P. Lalanne, Nano Lett. 15, 3439 (2015). "Simple Analytical Expression for the Peak-Frequency Shifts of Plasmonic Resonances for Sensing"

[3] K. G. Cognée, W. Yan, F. La China, D. Balestri, F. Intonti, M. Gurioli, A. F. Koenderink, and P. Lalanne, Optica 6, 269 (2019). "Mapping Complex Mode Volumes with Cavity Perturbation Theory"

[4] W. Yan, R. Faggiani, P. Lalanne, Phys. Rev. B **97** 205422 (2018). "Rigorous modal analysis of plasmonic nanoresonators"

Reversible Surface Charge Control through Supramolecular Chemistry

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The properties of nanomaterials are largely dependent on the size and morphology of nanoparticles, as well as on their organization within nanostructured materials. A large number of synthetic methods have been developed, which allow an exquisite degree of control over these parameters. One of the most important factors behind particle growth and interparticle interactions is the chemical composition of the nanoparticles' surface, which often involves the presence of organic ligands, usually surfactants or polymers. These ligands can be used to protect specific crystallographic facets in nanocrystals, to facilitate binding to other molecules or surfaces, but also to direct the assembly of the nanoparticles into well-defined nanostructures.
We describe an approach to regulate the surface charge on gold nanoparticles, using supramolecular chemistry. The strategy relies on the functionalization of AuNPs with negatively charged pyranines, which largely hamper their penetration in cells. Cellular uptake can be activated in situ through the addition of cationic covalent cages that specifically recognize the fluorescent pyranine dyes and counterbalance the negative charges. The high selectivity and reversibility of the host-guest recognition activates cellular uptake, even in protein-rich biological media, as well as its regulation by rational addition of either cage or pyranine.

References

[1] J. Mosquera, M. Henriksen-Lacey, I. García, M. Martínez-Calvo, J. Rodríguez, J.L. Mascareñas, L.M. Liz-Marzán, *J. Am. Chem. Soc.* **2018**, *140*, 4469-4472

Bio-inspired nanotechnology: from protein engineering to functional nanomaterials

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In our laboratory we apply bio-inspired approaches for the design and fabrication of hybrid functional nanostructures and biomaterials. We use repeat proteins as building blocks to develop modular versatile platforms for the fabrication of multiple protein-based hybrid functional nanostructures and biomaterials for their use in different applications including molecular electronics, optical plasmonics, catalysis, and photoactive systems among others. We combine rational protein engineering, structural biology and biophysical approaches to generate and characterize functional nanostructures and materials.

In addition, we develop new methodologies for the generation of versatile functional nanomaterials for biomedical applications including novel therapies, diagnosis and imaging approaches. We pay special attention to functionalization with biomolecules and to the generation of final formulations with optimal properties including their biocompatibility and stability, selective drug release and targeting capabilities, for being used under clinically relevant conditions.

References

[1] Aires, A., Llarena, I., Moller, M., Castro-Smirnov, J., Cabanillas-Gonzalez, J., Cortajarena, A. L., *Angew. Chem. Int. Ed.* (2019) 58: 6214-6219
[2] Mejias, S. H., Bahrami-Dizicheh, Z., Liutkus, M., Sommer, D. J., Astashkin, A., Kodis, G., Chirlanda, G., Cortajarena, A. L. *Chem. Comm.* (2019) 55: 3319-3322.
[3] J. López-Andarias, S.H. Mejías, T. Sakurai, W. Matsuda, S. Seki, F. Feixas, S. Osuna, C. Atienza, N. Martín, and A.L. Cortajarena. *Adv. Funct. Mat.* (2018) 28, 1704031
[4] A. Aires, J.F. Cadenas, R. Guantes, A.L. Cortajarena, *Nanoscale* (2017) 9: 13760-71

Figures

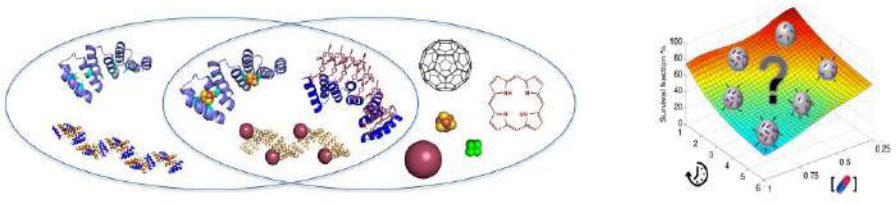

Figure 1. Biomolecular Nanotechnology: design of novel nanostructures and efficient nanomaterials.

Electronic correlations in excitations revealed by the scanning tunneling microscope

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Degenerate open-shell structures can undergo spin-flips when they are in contact with an electron reservoir giving rise to the Kondo effect. If the orbital structure is also degenerate, flips between different orbitals can be possible. This generally boosts the Kondo effect and changes the nature of the many-body ground state. When the degeneracy is lifted, inelastic effects can still connect the different state taking the extra energy from an applied bias. The consequence is that a new electron conduction channel opens when the applied bias matches the difference in energy between the non-degenerate levels. This has been shown for spins: lifting the spin degeneracy destroys the Kondo effect and two steps appear at positive and negative bias in the conductance. A similar effect takes place when the orbital degeneracy is lifted. Populating one level or another is like changing the sign of a pseudospin, also known as isospin. These orbitals show strong electronic correlations, because double occupancies lead to large charging energies. Hence, over the threshold to populate the higher-lying orbital, there is a competition to fill either orbital. This leads to a clear inelastic step in the conductance with orbital information. At positive bias a new channel is open that corresponds to a different orbital from the one at negative bias. This leads to spatially resolved steps in the conductance that are not symmetric with respect to bias. This isospin-flip inelastic effect has been recently observed in phthalocyanine molecules [1].

References

[1] Jens Kügel et al. Phys. Rev. Lett. **121**, 226402 (2018)

Visualization of multifractal superconductivity in a two-dimensional transition metal dichalcogenide in the weak-disorder regime

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Eigenstate multifractality is a distinctive feature of non-interacting disordered metals close to a metal-insulator transition, whose properties are expected to extend to superconductivity. While multifractality in three dimensions (3D) only develops near the critical point for specific strong-disorder strengths, multifractality in quasi-two dimensional (2D) systems with spin-orbit coupling is expected to be observable even for weak disorder. Here we investigate the impact of multifractality on the superconducting state [1] of an intrinsic weakly disordered single-layer of $NbSe_2$ by means of low-temperature scanning tunneling microscopy/spectroscopy (STM/STS) [2]. The superconducting gap, characterized by its width, depth and coherence peaks amplitude, shows characteristic spatial single-wavelength modulation nearly coincident with the periodicity of the quasiparticle interference pattern observed at the Fermi energy. Spatial inhomogeneity of the superconducting gap width, which is proportional to the local order parameter in the weak disorder regime, shows a characteristic log-normal statistical distribution as well as a power-law decay of the two-point correlation function, in agreement with our theoretical model. This novel state is universal and governs the properties of even weakly disordered 2D superconductors with spin-orbit coupling. This offers a novel platform to tune and ultimately control superconductivity in novel 2D quantum materials.

References

[1] M. M. Ugeda, et al., Nature Physics 12, 92 (2016).
[2] C. Rubio-Verdú, et al, submitted (2019).

Figures

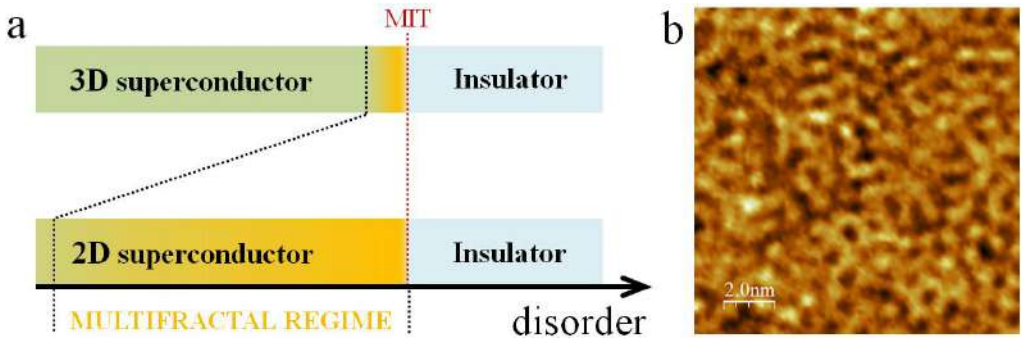

Figure 1. a. Sketch of the extent of the multifractal regime in the superconducting state in 3D and 2D. b. Spatial distribution of the superconducting order parameter in a 12 nm x 12 nm region of single-layer $NbSe_2$.

Tunable Multispectral Photonic Stopbands Based on Structurally Engineered Nanoporous Anodic Alumina

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The control of light–matter interactions at the nanoscale with precision is of fundamental importance for the development of advanced photonic devices and new photonic applications. Nanoporous anodic alumina (NAA) is an interesting base material for the fabrication of photonic structures. NAA is obtained by the electrochemical oxidation of aluminum that under specific conditions presents a self-ordered hexagonal pore distribution of parallel cylindrical nanopores [1-2]. The fabrication is cost-effective and fully scalable process compatible with conventional micro- and nanofabrication approaches.

NAA has been used to fabricate photonic crystals with the aim to control the properties of light when the electromagnetic waves travel across the matter. The photonic crystals are periodic structures with a periodic variation of the refractive index. The periodicity of these structures defines regions of the spectrum where the propagation of light is forbidden (photonic stopbands).

The fabrication of photonic structures (PSs) with multiple narrow photonic stopbands at different spectral positions (UV-Vis-NIR) remains a challenge These PSs can be obtained by averaging the sum of multiple sinusoidal waves into a single complex waveform, which is subsequently translated into anodization profiles to engineer the nanoporous structure of these PSs in depth. Each sinusoidal wave determines the spectral position and the reflectance amplitude of a forbidden photonic band or photonic stopband. Multiple-band NAA structures have interesting applications such as optical encoding tags [3], optical sensing [4], photonics [5] and photovoltaics. In this presentation, we present a comprehensive study of different photonic structures based on single and multiple periodic structures with sinusoidal profiles both in an overlapped and in a stacked configuration. We analyze different technological parameters and its effect on the structure and the stopbands. Finally, we will present some examples of sensing and optical encoding.

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References

[1] A Santos, A., Formentín, P., Pallarès, J., Ferré-Borrull, J., Marsal, L.F., (2011) Journal Electroanalytical Chemistry 655 (1), 73-78.
[2] Santos, A., Vojkuvka, L., Alba, M., Balderrama, V.S., Ferré-Borrull, J., Pallarès, J., Marsal, L.F., (2012) Physica Status Solidi (A) Applications and Materials Science, 209 (10), 2045-2048.
[3] Santos, A., Law, C.S., Pereira, T., Losic, D., (2016) Nanoscale 8(15), 8091-8100
[4] Acosta, L.K., Bertó-Roselló, F., Xifre-Perez, E., Santos, A., Ferré-Borrull, J., Marsal, L.F., (2019) ACS Applied Materials and Interfaces, 11 (3), 3360-3371.
[5] Kumeria, T., Santos, A., Rahman, M.M., Ferré-Borrull, J., Marsal, L.F., Losic, D., (2014) ACS Photonics, 1 (12), pp. 1298-1306.

Quantum nanophotonics: using nanostructures to manipulate photons

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With technological advances allowing the fabrication of smaller and smaller components for electronic and optical processing it is important that we understand and embrace the possibilities of combining the use of quantum technologies in the nanosciences. In this talk I will present three recent results of my research group which showcase the possibilities of applying the concepts of Quantum Optics and Quantum Information in Nanophotonics, with particular emphasis in sensing and metrology applications. In particular I will show our recent efforts in using quantum metrology to perform measurements of the optical rotatory dispersion of chiral molecules, how photonic quantum states can be engineered to interact with structures smaller than the wavelength of light and to control the state of levitated nanoparticles.

References

[1] Büse, A., Juan, M. L., Tischler, N., D'Ambrosio, V., Sciarrino, F., Marrucci, L., & Molina-Terriza, G. (2018). Symmetry protection of photonic entanglement in the interaction with a single nanoaperture. Physical review letters, 121(17), 173901.

[2] Tischler, N., Krenn, M., Fickler, R., Vidal, X., Zeilinger, A., & Molina-Terriza, G. (2016). Quantum optical rotatory dispersion. Science advances, 2(10), e1601306.

[3] Juan, M. L., Bradac, C., Besga, B., Johnsson, M., Brennen, G., Molina-Terriza, G., & Volz, T. (2017). Cooperatively enhanced dipole forces from artificial atoms in trapped nanodiamonds. *Nature Physics*, *13*(3), 241.

Strategies for Shape-Controlled Magnetic Iron Oxide Nanoparticles for biomedical applications

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The improvement of the performance of magnetic iron oxide nanoparticles in their different applications requires the design of more complex synthetic nanostructures, uniform in size and with morphologies different from the spherical one (Fig. 1). We critically analyze the synthesis routes for the production of uniform anisometric magnetite/maghemite nanoparticles with different morphologies like cubes, rods, disks, flowers and many others, such as hollow spheres, worms, stars or tetrapods, detecting the key parameters governing the production of these nanoparticles with particular emphasis in the role of the ligands in the final nanoparticle morphology [1]. The main structural and magnetic features as well as the nanotoxicity as a function of the nanoparticle morphology are also described. Finally, the impact of each morphology on the different biomedical applications (hyperthermia, magnetic resonance imaging and drug delivery) are analyzed in detail [2, 3].

References

[1] Roca et al. Advanced Drug Delivery Reviews, December 2018, DOI: 10.1016/j.addr.2018.12.008.
[2] Del Sol-Fernandez et al., ACS Appl. Mater. Interfaces 2019, 11, 26648−26663
[3] Serantes et al, Phys. Chem. Chem. Phys., 2018, 20, 30445.

Figures

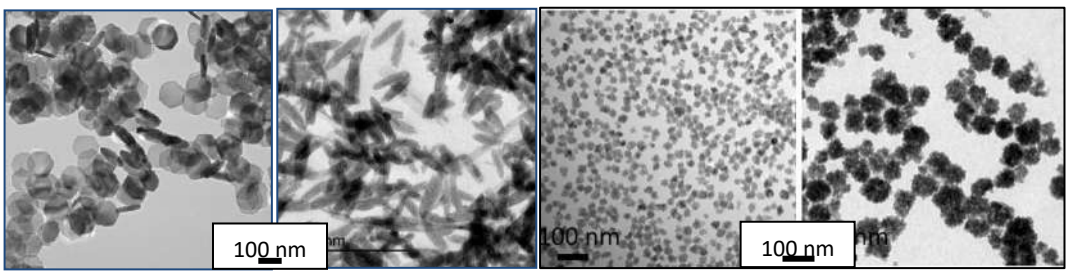

Figure 1. Magnetic iron oxide nanoparticles with different morphologies.

Towards wafer-scale fabrication of graphene based electronic, photonic and sensor devices

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Graphene based electronic, photonic and sensor devices have attracted significant interests because of their outstanding properties. However, for commercialization of these devices the large volume production, i.e. wafer-scale processing, needs to be solved. While wafer scale growth of graphene and related 2D materials has been demonstrated by means of chemical vapor deposition or similar methods, the transfer of such grown 2D layers to target substrates still faces severe challenges related to contamination, mechanical stress and reproducibility. In addition, defining and controlling quality, yield and reproducibility of (opto-)electronic devices is at a very early stage.
In this presentation I will discuss approaches, challenges and possible solutions for the wafer scale integration of graphene based electronic and photonic devices. The performance of such devices will be compared to chip scale production and the current limitations for yield, device to device variation and reproducibility will be discussed.

References

[1] D. Schall et al. *Graphene photodetectors with a bandwidth> 76 GHz fabricated in a 6" wafer process line.* J. Phys. D: Appl. Phys 50 (124004), 124004 (2017).
[2] G Ruhl et al. *The integration of graphene into microelectronic devices.* Beilstein Journal of Nanotechnology 8 (1), 1056-1064 (2017).
[3] D. Neumaier, S. Pindl and M. Lemme *Integrating Graphene into Semiconductor Fabrication Lines.* Nature Materials 18, 525–529 (2019).

Figures

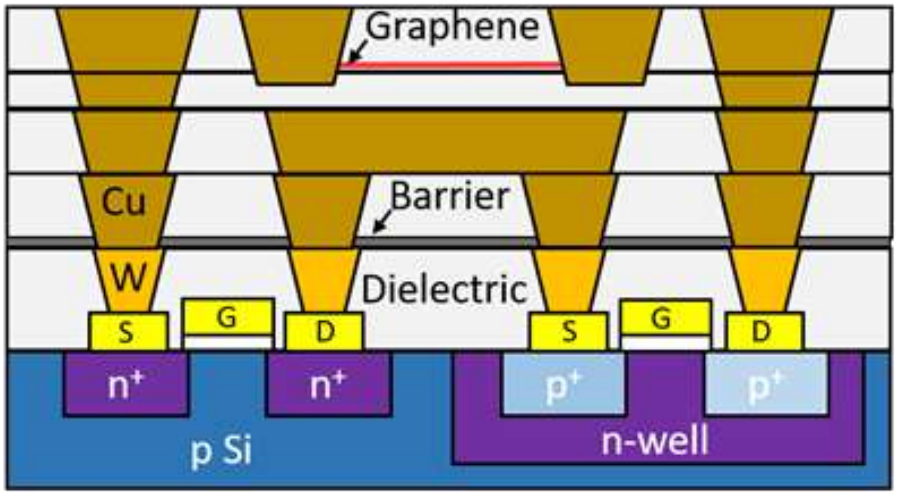

Figure 1. Possible integration scheme of graphene into a silicon CMOS platform at the back-end-of-the-line, as it could be used for graphene based Hall Sensors.

Understanding the origin of Charge Density Waves from First-Principles: clearing misconceptions and explaining real materials

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The concept of a Charge Density Wave (CDW), a periodic modulation of the electronic charge density of a crystal with a period longer than original periodicity of the underlying crystalline lattice, is widespread in condensed matter physics, particularly in the context of metals with low dimensional electronic character. The Peierls' and Frölich's picture of CDW originating from an instability of the 1D electron gas, followed by a periodic lattice distortion (PLD) and the development of a metal-insulator transition, was at the origin of the CDW concept, and provided a clear guideline to search for materials exhibiting it and for the interpretation of the experimental observations [1]. However, we know today that many of the CDW instabilities observed many materials are not due to a Peierls instability, but have other physical origins [2]. Nevertheless, the Peierls mechanism cannot be discarded a priori as the origin of the CDW and the PLD in a given material.

In this talk, I will show how First-Principles calculations (within the formalism of Density Functional Theory – DFT) can help in sorting out the physical origin of the appearance of CDW in specific materials. I will show how the Peierls picture describes very accurately the observation of CDWs in the blue bronzes, by analyzing the Lindard response function computed from DFT [3]. However, for the layered transition metal dichalcogenides (TMDs), in which the CDW were observed long ago in layered 3D crystals, and which are currently the subject of renewed interest in their single- and few-layer 2D counterparts, our calculations show that the Peierls mechanism is not responsible for the appearance of the CDW. We analyze in detail the situation for several of these TMDs, like $NbSe_2$ [4,5], $TiSe_2$ [6] and $TiTe_2$ [7].

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References

[1] J.-P. Pouget, Comptes Rendues Physique 17 332 (2016)
[2] M. D. Johannes and I. I. Mazin, Phys. Rev. B 77, 165135 (2008)
[3] B. Guster, M. Pruneda, P. Ordejón, E. Canadell and J. -P. Pouget, Phys. Rev. Materials 3, 055001 (2019).
[4] J. Silva-Guillén, F. Guinea, P. Ordejón, E. Canadell, 2D Materials 3, 035028 (2016).
[5] B. Guster, C. Rubio-Verdú, R. Robles, J. Zaldívar, P. Dreher, M. Pruneda, J. A. Silva-Guillén, D.-J. Choi, J. I. Pascual, M. M. Ugeda, P. Ordejón, and E. Canadell, Nano Letters 19, 3027 (2019)
[6] B. Guster, E. Canadell, M. Pruneda and P. Ordejón, 2D Materials 5 025024 (2018)
[7] B. Guster, R. Robles, M. Pruneda, E. Canadell and P. Ordejón, 2D Materials 6 015027 (2019)

Magnetism in graphene nanoribbons

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Graphene can spontaneously develop intrinsic paramagnetism. Crucial examples are the magnetization of zig-zag edges in graphene, or the emergence of paramagnetism in open shell graphene nanostructures. I will show that graphene nanoribbons (GNR), fabricated with atomic precision on a metal surface exhibit fingerprints of pi-paramagnetism on a metal surface, which can be detected and spatially localized using low temperature scanning tunneling [1].

Single electron spins emerge localized at certain zigzag sites of the carbon backbone. Their presence could be detected and mapped by spatially resolving the zero-energy resonance due to the Kondo effect (see figure below). We found that near-by spins are coupled into a singlet ground state and quantify their exchange interaction via singlet-triplet inelastic electron excitations. Theoretical simulations picture how electron correlations result in spin-polarized radical states with the experimentally observed spatial distributions. Extra hydrogen atoms bound to radical sites quench their magnetic moment and switch the spin of the nanostructure in half-integer amounts.

I will also review other methods for activating magnetic ground states in graphene. The simplest one is to incorporate magnetic molecular species into a ribbon using on-surface synthesis routes (see included image of a Fe porphyrin contacted to chiral nanoribbons). We prove that the molecular spin survives in the ribbon by using spin-excitation inelastic spectroscopy [2]. By proper selecting the position of the halogen functionalization, we fabricated linear GNR-FeTPP-GNR structures and performed electronic transport measurements [3], detecting spin-excitation fingerprints in transport mode.

References

[1] J. Li, S. Sanz, M. Corso, D.J. Choi, D. Peña, T. Frederiksen, J.I. Pascual, "*Single Spin Localization and Manipulation in Graphene Open-Shell Nanostructures*", Nature Communications 10, 200 (2019).

[2] J. Li, N. Merino-Díez, E. Carbonell-Sanromà, M. Vilas-Varela, D. G. de Oteyza, D. Peña, M. Corso, and J.I. Pascual, "*Survival of spin state in magnetic porphyrins contacted by graphene nanoribbons*" Science Advances 4, eaaq0582 (2018)

[3] J. Li, N. Friedrich, N. Merino-Díez, D. G. de Oteyza, D. Peña, D. Jacob, and J.I. Pascual, "*Electrically Addressing the Spin of a Magnetic Porphyrin through Covalently Connected Graphene Electrodes*", Nano Letters 19, 3288 (2019).

Figures

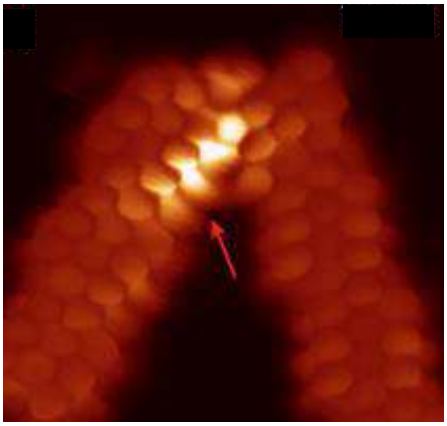

Figure 1. Single spin localization in a graphene nanostructure [1]

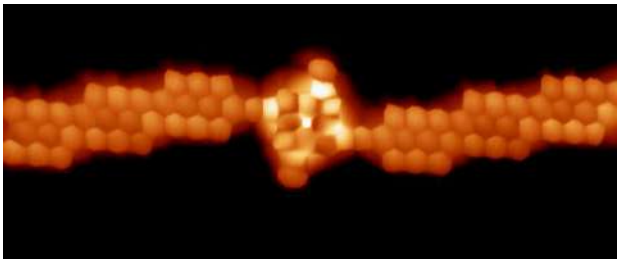

Figure 2. Two chiral GNRs contacting a single Iron Porphyrin molecule [3]

Building graphene materials by combining organic synthesis and surface science

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The development of atomic force microscopy (AFM) and scanning tunnelling microscopy (STM) with functionalized tips has allowed the visualization of molecules adsorbed on different surfaces with submolecular resolution. This advance, together with the possibility to induce on-surface chemical reactions, opens up exciting applications in chemistry and materials science.[1]
In this talk, I will comment on how these breakthroughs in AFM/STM, in combination with organic synthesis, allowed us to obtain and characterize graphene-like nanostructures. In particular, I will discuss the synthesis and characterization of nanographenes such as cloverphenes (Fig 1A), dendripenes (Fig 1B)[2] and kekulene (Fig 1C). In addition, I will comment on the preparation of porous nanographenes (Fig 1D-E)[3] by combining solution chemistry and on-surface synthesis, as well as large acenes (Fig 1F)[4] and our first efforts towards the on-surface generation of cyclacenes (Fig 1G).[5]

References

[1] L. Gross, B. Schuler, N. Pavliček, S. Fatayer, Z. Majzik, N. Moll, D. Peña, G. Meyer *Angew. Chem. Int. Ed.* **2018**, *57*, 3888.
[2] M. Vilas-Varela, S. Fatayer, Z. Majzik, D. Pérez, E. Guitián, L. Gross, D. Peña *Chem. Eur. J.* **2018**, *24*, 17697
[3] J. Hieulle, E. Carbonell-Sanromà, M. Vilas-Varela, A. García-Leuke, E. Guitián, D. Peña, J. I. Pascual *Nano Lett.* **2018**, *18*, 418.
[4] J. Krüger, F. García, F. Eisenhut, D. Skidin, J. M. Alonso, E. Guitián, D. Pérez, G. Cuniberti, F. Moresco, D. Peña *Angew. Chem. Int. Ed.* **2017**, *56*, 11945.
[5] F. Schulz, F. García, K. Kaiser, D. Pérez, E. Guitián, L. Gross, D. Peña *Angew. Chem. Int. Ed.* **2019**, *58*, 9038.

Figures

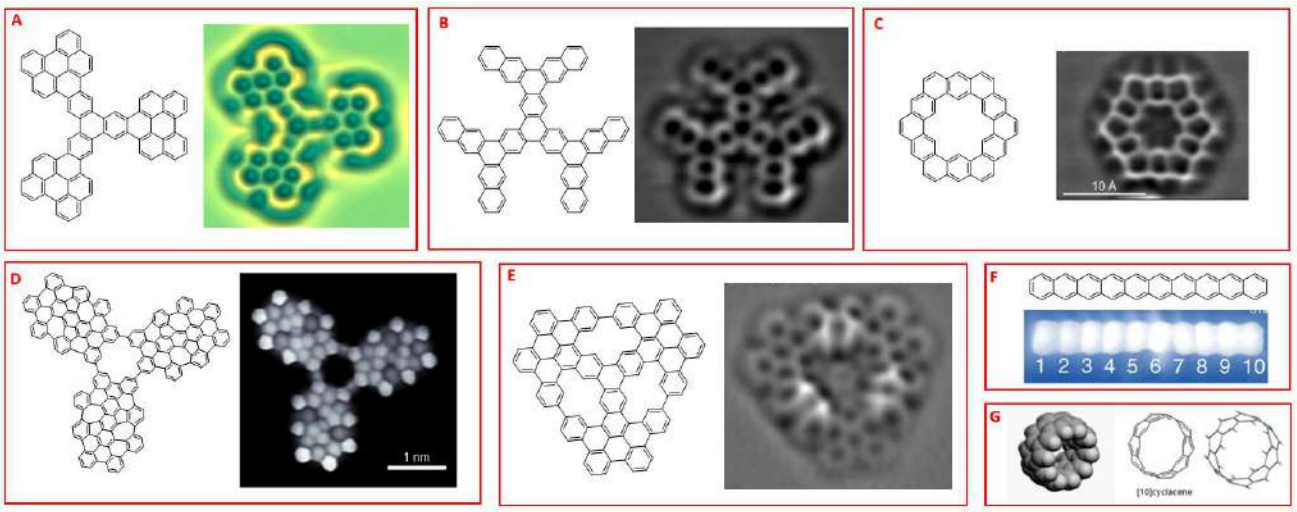

Figure 1. Selected examples of graphene molecules described in this lecture.

Novel DNA-Based Molecules and Their Charge Transport Properties

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Charge transport through molecular structures is interesting both scientifically and technologically. To date, DNA is the only type of polymer that transports significant currents over distances of more than a few nanometers in individual molecules. Nevertheless and in spite of large efforts to elucidate the charge transport mechanism through DNA a satisfying characterization and mechanistic description has not been provided yet. For molecular electronics, DNA derivatives are by far more promising than native DNA due to their improved charge-transport properties.

In recent years we have invested great efforts to address the above issues. Measuring the charge transport in DNA was elusive due to great technical difficulties leading to various results. We recently devised an experiment in which double-stranded DNA is well positioned between metal electrodes. Electrical measurements give surprisingly high currents over 100 base-pairs (~30 nm) elevated from the surface. The temperature dependence indicates backbone-related band-like transport.

In collaboration with the Kotlyar group, We were also able to synthesize and measure long (hundreds of nanometers) DNA–based derivatives that transport significant currents when deposited on hard substrates. Among the molecules, metal containing DNA, which is true metal-organic hybrid, a smooth and thin metal coated DNA and G-quadruplex DNA.

Step by step we improve the synthesized constructs and the measurement methods of single DNA-based molecules. I will present new and surprising results on dsDNA molecules. I will present new DNA-based molecules and report on our measurements of their properties.

References

[1] "Direct measurement of electrical transport through DNA molecules", Danny Porath, Alexey Bezryadin, Simon de Vries and Cees Dekker, Nature 403, 635 (2000).

[2] "Charge Transport in DNA-based Devices", Danny Porath, Rosa Di Felice and Gianaurelio Cuniberti, Topics in Current Chemistry Vol. 237, pp. 183-228 Ed. Gary Shuster. Springer Verlag, 2004.

[3] “Direct Measurement of Electrical Transport Through Single DNA Molecules of Complex Sequence”, Hezy Cohen, Claude Nogues, Ron Naaman and Danny Porath, PNAS 102, 11589 (2005).

[4] “Long Monomolecular G4-DNA Nanowires”, Alexander Kotlyar, Nataly Borovok, Tatiana Molotsky, Hezy Cohen, Errez Shapir and Danny Porath, Advanced Materials 17, 1901 (2005).

[5] “Electrical characterization of self-assembled single- and double-stranded DNA monolayers using conductive AFM”, Hezy Cohen et al., Faraday Discussions 131, 367 (2006).

[6] “High-Resolution STM Imaging of Novel Poly(G)-Poly(C)DNA Molecules”, Errez Shapir, Hezy Cohen, Natalia Borovok, Alexander B. Kotlyar and Danny Porath, J. Phys. Chem. B 110, 4430 (2006).

[7] "Polarizability of G4-DNA Observed by Electrostatic Force Microscopy Measurements", Hezy Cohen et al., Nano Letters 7(4), 981 (2007).

[8] “Electronic structure of single DNA molecules resolved by transverse scanning tunneling spectroscopy”, Errez Shapir et al., Nature Materials 7, 68 (2008).

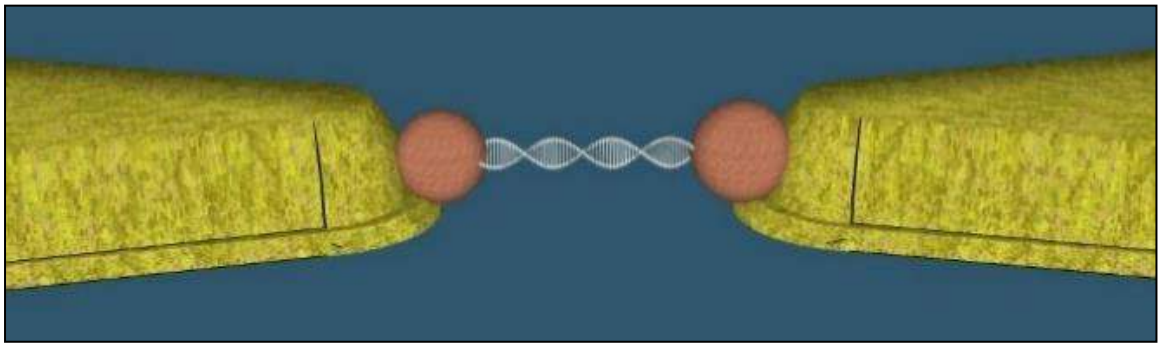
[9] “A DNA sequence scanned”, Danny Porath, Nature Nanotechnology 4, 476 (2009).

[10] “The Electronic Structure of G4-DNA by Scanning Tunneling Spectroscopy”, Errez Shapir, et.al., J. Phys. Chem. C 114, 22079 (2010).

[11] “Energy gap reduction in DNA by complexation with metal ions”, Errez Shapir, G. Brancolini, Tatiana Molotsky, Alexander B. Kotlyar, Rosa Di Felice, and Danny Porath, Advanced Maerials 23, 4290 (2011).
[12] "Quasi 3D imaging of DNA-gold nanoparticle tetrahedral structures", Avigail Stern, Dvir Rotem, Inna Popov and Danny Porath, J. Phys. Cond. Mat. 24, 164203 (2012).
[13] "Comparative electrostatic force microscopy of tetra- and intra-molecular G4-DNA", Gideon I. Livshits, Jamal Ghabboun, Natalia Borovok, Alexander B. Kotlyar, Danny Porath, Advanced materials 26, 4981 (2014).
[14] "Long-range charge transport in single G4-DNA molecules", Gideon I. Livshits et. al., Nature Nanotechnology 9, 1040 (2014).
[15] "Synthesis and Properties of Novel Silver containing DNA molecules", Gennady Eidelshtein et. al., Advanced Materials 28, 4839 (2016).
[16] "Highly conductive thin uniform gold-coated DNA nanowires", Avigail Stern et. al., Advanced Materials 30, 1800433 (2018).
[17] “Advances in Synthesis and Measurement of Charge Transport in DNA-Based Derivatives”. R. Zhuravel, A. Stern, N. Fardian-Melamed, G. Eidelshtein, L. Katrivas, D. Rotem, A. Kotlyar and D. Porath, Advanced Materials 30, 1706984 (2018).
[18] “Scanning Tunneling Microscopy and Spectroscopy of Novel Silver-Containing DNA Molecules”, Natalie Fardian-Melamed, Gennady Eidelstein, Dvir Rotem, Alexander Kotlyar and Danny Porath, Advanced Materials, Article Number: 1902816 (2019).

Figures

Figure 1. Calibri 10



Surface nanopatterning and 3d architecture of cell aggregation

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Living systems can be envisioned as multicellular networks that maintain a continuous efficient flow of information within and between cells and with the surrounding environment. In pluricellular organisms, cell-to-cell communication is crucial for the adaptation to a community environment, allowing the specialization into differentiated tissues and the preservation of homeostasis and correct function. Mechanical and chemical signaling are effectively combined to regulate the transfer of information between cells. During morphogenesis, dynamic adhesion mechanisms, together with the associated regulatory signaling pathways, define tissue differentiation and architecture. Mesenchymal cell condensation is a prevalent morphogenetic transition regulated by cell adhesion in which mesenchymal stem cells (MSCs) gather together forming intimate cell-to-cell contacts. In osteochondral development, condensation is concurrent to the formation of an extensive gap junctional communication network which provide intercellular and cell-matrix communication. Although previous studies have related gap junction intercellular communication (GJIC) with matrix-associated proteins, little is known about the way the environment modulates the formation of such a GJ communication network and its implications in tissue architecture and function. We have used nanopatterns of the cell adhesive arginine-glycine-aspartic acid (RGD) peptide to tailor local surface adhesiveness at the nanoscale and study their influence in the cell aggregation and the establishment of intercellular communication during mesenchymal condensation.

References

[1] Lagunas et al. Nano Res. DOI: 10.1007/s12274-014-0406-2 (2014)
[2] Casanellas et al. J. Vis. Exp. DOI: 10.3791/56347 (2018)
[3] Lagunas et al. Nano Res. DOI: 10.1007/s12274-016-1382-5 (2017)
[4] Casanellas et al. Biomimetics DOI: 10.3390/biomimetics4020043 (2018)

The Interplay of Metasurfaces and Metamaterials

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Three dimensional interconnected periodic networks made from plasmonic metals are interesting implementations of optical metamaterials that mold the flow of light in unusual ways. In particular, the templating of self-assembled polymer morphologies allows to access periodic lattice dimensions below 100 nm for the creation of metamaterials with an optical response at visible wavelengths [1,2]. In these lattices, light couples into plasmon-polariton modes which propagate across the metamaterial, coupling out into optical modes on the other side. Evidently, the in- and outcoupling at the metamaterial-surfaces play an important role in the photonic-plasmonic mode coupling.

In this presentation, the role of terminating metasurfaces of 3D metamaterials is discussed. Minute details of these surfaces can substantially modify the photonic-plasmonic mode coupling. In particular these surfaces can break the bulk symmetry and lead to localized plasmonic surface modes that do not exist in the bulk [3]. The results of our study allow to better understand the optical behavior of self-assembled metamaterials and guides their design.

References

[1] A 3D Optical Metamaterial Made by Self-Assembly, *Silvia Vignolini, Nataliya A. Yufa, Pedro S. Cunha, Stefan Guldin, Ilia Rushkin, Morgan Stefik, Kahyun Hur, Ulrich Wiesner, Jeremy J. Baumberg, Ullrich Steiner*, Advanced Materials *24*, OP23-OP27 (2012)

[2] Optical Properties of Gyroid Structured Materials: From Photonic Crystals to Metamaterials, *James A. Dolan, Bodo D. Wilts, Silvia Vignolini, Jeremy J. Baumberg, Ullrich Steiner, Timothy D. Wilkinson*, Advanced Optical Materials *3*, 12-32 (2015)

[3] Metasurfaces Atop Metamaterials: Surface Morphology Induces Linear Dichroism in Gyroid Optical Metamaterials, *James A. Dolan, Raphael Dehmel, Angela Demetriadou, Yibei Gu, Ulrich Wiesner, Timothy D. Wilkinson, Ilja Gunkel, Ortwin Hess, Jeremy J. Baumberg, Ullrich Steiner, Matthias Saba, Bodo D. Wilts*, Advanced Materials *31*, 1803478 (2019)

Figures

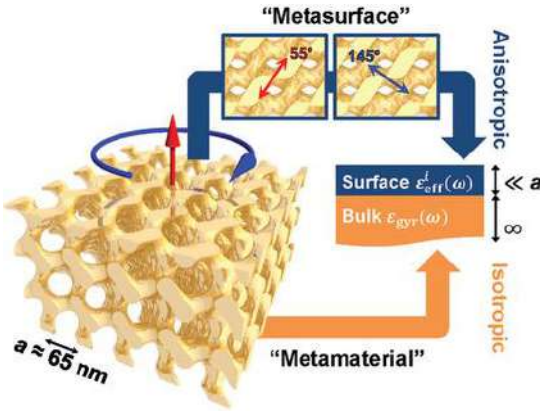

Figure 1. Interplay of metasurfaces and 3D metamaterials

INVITED SPEAKERS contributions

DNA origami nanotools for nanophotonics

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The field of nanophononics is primarily concerned with manipulating light at the nanoscale. The key elements in this field are optical antennas [1], which represent the counterparts of radio and microwave antennas within the visible spectrum. These antennas are mostly built from metallic nanoparticles whose localized surface plasmon resonances enable the control of light fields in the sub-wavelength range. Currently, optical antennas are being studied for a wide range of applications such as optical communications, light harvesting, enhanced spectroscopies and sensing.
In this contribution, we will focus on an alternative bottom-up self-assembly approach for the fabrication of optical antennas based on colloidal metallic nanoparticles: the DNA origami technique [2]. We will show how this method can outperform top-down fabricated optical antennas. In addition, we will also study how DNA origami based optical antennas can enhance fluorescence [3,4], direct emission [5], shift the apparent emission center [6] and be combined with graphene [7], natural light harvesting complexes [8] and lithographic structures [9].

References

[1] Novotny, L.; Van Hulst, N. *Nat. Photonics* **2011**, 5 (2), 83–90.
[2] Rothemund, P. W. K. *Nature*. **2006**, pp 297–302.
[3] Acuna, G. P.; Möller, F. M.; Holzmeister, P.; Beater, S.; Lalkens, B.; Tinnefeld, P. *Science (80-.).* **2012**, *338* (6106), 506–510.
[4] Puchkova, A.; Vietz, C.; Pibiri, E.; Wünsch, B.; Sanz Paz, M.; Acuna, G. P.; Tinnefeld, P. *Nano Lett.* **2015**, *15* (12), 8354–8359.
[5] Hübner, K.; Pilo-Pais, M.; Selbach, F.; Liedl, T.; Tinnefeld, P.; Stefani, D.; Acuna, G.P. *Nano Lett.* **2019** (under review).
[6] Raab, M.; Vietz, C.; Stefani, F. D.; Acuna, G. P.; Tinnefeld, P. *Nat. Commun.* **2017**, *8* (1), 13966.
[7] Kaminska, I.; Bohlen, J.; Rocchetti, S.; Selbach, F.; Acuna, G. P.; Tinnefeld, P. *Nano Lett.* **2019**.
[8] Kaminska, I.; Bohlen, J.; Mackowski, S.; Tinnefeld, P.; Acuna, G. P. *ACS Nano* **2018**, *12* (2), 1650–1655.
[9] Pibiri, E.; Holzmeister, P.; Lalkens, B.; Acuna, G. P.; Tinnefeld, P. *Nano Lett.* **2014**, *14* (6), 3499–3503.

Figures

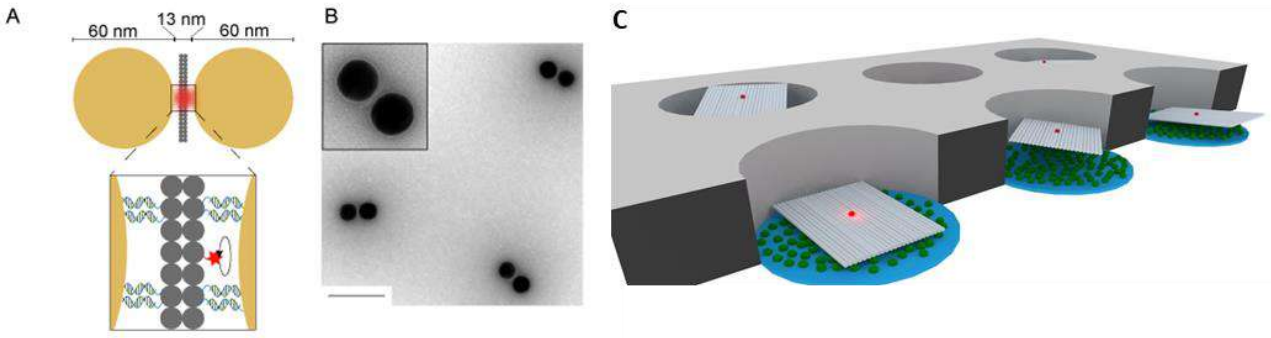

Figure 1. (A) Sketch of an optical antena dimer structure composed of two gold nanoparticles self-assembled onto a rectangular DNA origami. The inset depicts a close-up of the NP gap where a single single Cy5 fluorophore is incorporated. (B) TEM images of the dimer structures (scale bar is 200 nm). (C) Combination of DNA origami structures (grey rectangles) with zero-mode waveguides (also termed nanoapertures).

Probing the magnetism of topological end-states in armchair graphene nanoribbons

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Materials purely made up of non-magnetic atoms can display magnetic properties. One such example are aromatic hydrocarbon structures. Following Lieb´s theorem, if the number of atoms in each carbon sublattice is different, the molecular structure will hold a net spin. However, even in the absence of net spin, polyradicals can be generated on graphitic structures subject to particular edge topologies. In addition to the edge topologies, also the structure´s size determines the presence or absence of such radical states, whose corresponding spin, if present, is furthermore predicted to display a specific relative alignment. These interesting predictions are hard to verify because of the difficulty in the synthesis of appropriate nanographytic structures with atomic precision. In this respect, on-surface synthesis under vacuum conditions has appeared as an extremely promising approach. Making use of it, we have synthesized a variety of nanosized aromatic hydrocarbon structures with well-determined shapes and sizes, including graphene nanoribbons with different edge morphologies, widths and lengths. For the particular case of 5 atoms wide armchair graphene nanoribbons we describe, based on scanning tunneling microscopy and spectroscopy, combined with theoretical calculations, their electronic properties and the magnetism associated to its topologic end-states.

Figures

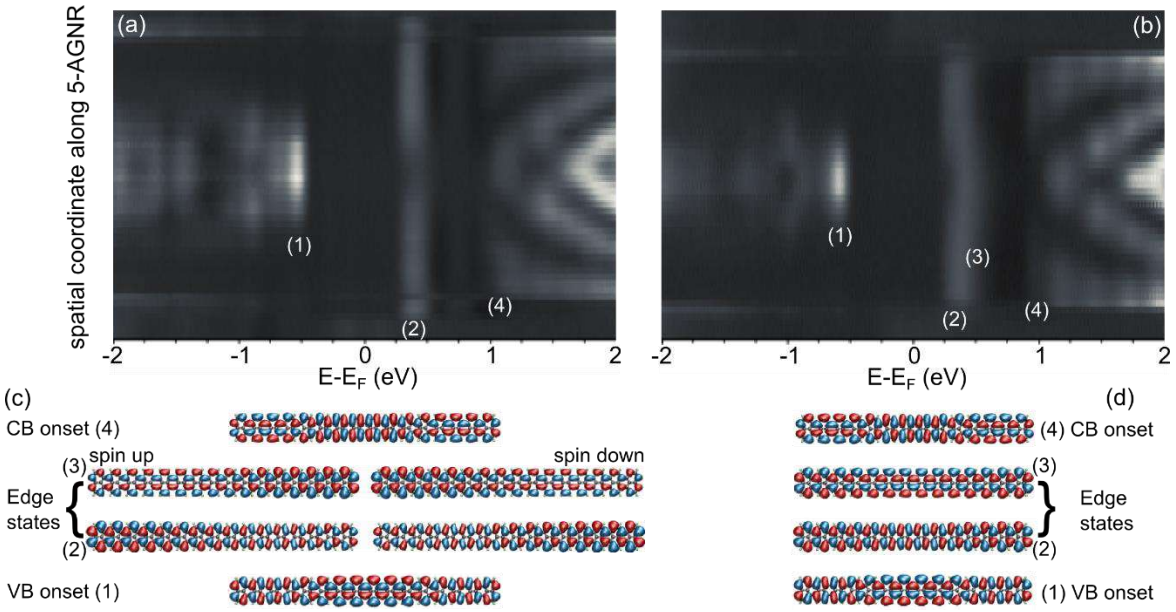

Figure 1. Size-dependent spin polarization of edge states in 5-aGNRs. (a) Stacked dI/dV point spectra along a 5-aGNR made up by (a) 8 and (b) 7 reactant molecules, as well as the corresponding calculated wave functions for the edge states, valence band and conduction band onset [(c) and (d)] appropriately labelled in upper and lower panels for correspondence.

Coupling X-ray spectroscopy and Scanning Probe Microscopy

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Abstract

Non-destructive tools providing elemental and chemical analysis at high resolution are necessary for life and material sciences. For example, electronics or glass industry needs in-lab tools for material processing and control (RRAM, FeRAM, smart materials, solar cells….). From the growth of interest for nanosciences, new tools have emerged to analyze matter at the nanoscale. That is the reason why focused incident beams were developed and are nowadays available on many set-ups. Combination of multiple characterization studies has become a necessity to be able to elaborate more complex materials and structures with a high quality control level. However, on most equipments, analysis is made at some area on the sample that is very difficult to refind using another characterization technique, especially when working at a nanometric scale.

To overcome this difficulty, the coupling and alignment of various analysis techniques and tools at the same point on a sample at this scale is now a reality even if it is still a sensitive issue. Among the recent progresses in this field, the coupling of near-field microscopy with other techniques has received great consideration. Because X-Ray spectroscopies are able to deliver very accurate chemical and strucutral information at the atomic scale, they were ideal candidates for this purpose. The idea of coupling both techniques emerged [1-4]. This lecture aims to give an overview of the most significant results that have been published since about ten years in this context.

References

[1] K. Tsuji et al., Surf. and Interface Analysis **27**, 132 (1999)

[2] A. Saito et al., Journ. of Synchrotron Radiation **13**, 216 (2006)

[3] V. Rose et al, Appl. Phys. Lett. **92**, 193510 (2008)

[4] S. Larcheri et al, Rev. of Scientific Instruments **79**, 013702 (2008)

Light in correlated disordered media

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Disorder has been considered a major drawback in any optical material design since the presence of uncontrolled scattering sources can spoil the intended performance of virtually any design. This fact is particularly evident in photonic crystals because the very existence of a photonic band structure relies on an exact translation invariance. However, disorder is not always as harming as one might expect. In particular, optical structures with correlated disorder can exhibit a rich variety of light transport regimes.

In this contribution, we will discuss some of the results obtained in this field in the last years. Stealth hyperuniform (SHU) structures [1] have been shown to exhibit a well defined and substantially wide photonic gap despite being disordered [2]. Furthermore, this behavior is not exclusive of this particular kind of correlated disorder but appears in wider classes of correlated disordered photonic structures [3].

In the case of two dimensional SHU optical materials, it has been shown that several fundamentally different light transport regimes can emerge and be controlled depending on correlation degree, materials and wavelength [4]. These range from the purest transparency (stealthiness) to isotropic photonic bandgaps passing through regimes of light diffusion and strong Anderson localization. All of them are accessible in a relatively narrow wavelength span.

It is particularly relevant to have designer rules for three dimensional optical materials showing Anderson localization. In this regard, we will discuss the strong numerical evidence found in correlated disordered three dimensional photonic networks [5].

References

[1] R.D. Batten, F.H. Stillinger, and S. J. Torquato, App.Phys. 104, 033504 (2008).
[2] M. Florescu, S. Torquato, and P. J. Steinhardt, PNAS 106, 20658 (2009).
[3] L. S. Froufe-Pérez, M. Engel, P. F. Damasceno, N. Muller, J. Haberko, S. C. Glotzer, and F. Scheffold, Phys. Rev. Lett., 117, 053902 (2016).
[4] L. S. Froufe-Pérez, M. Engel, J.J. Sáenz, F. Scheffold, PNAS 114, 9570-9574 (2017).
[5] J. Haberko, L. S. Froufe-Pérez, and F. Scheffold, arXiv:1812.02095 (2018).

Optomechanical interaction driven by complexity

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Precision is a virtue in science in general and nanotechnology in particular where carefully fabricated nanometer-scale devices hold great promise in both classical and quantum regimes. Ground-state cooling or phonon amplification require, for example, a sideband resolved photon-phonon coupling where unavoidable imperfections often impose severe performance limits. However, imperfection and disorder are ubiquitous in Nature and emerge with a role particularly important in nanoscale devices.

In this talk, I will explore the limits imposed by imperfection in different nanodevices, but not only. In certain cases, disorder may be invoked to enable new functionalities and can be exploited to enhance the light-matter interaction in different fields of nanotechnology such as quantum photonics [1], nonlinear photonics [2], phononics [2] and optomechanics [3].

References

[1] P.D. Garcia, P Lodahl. Physics of Quantum Light Emitters in Disordered Photonic Nanostructures. **Annalen der Physik** 529, 1600351 (2017).
[2] G Arregui, D Navarro-Urrios, N Kehagias, CMS Torres, PD Garcia. All-optical radio-frequency modulation of Anderson-localized modes. **Physical Review B** 98 (18), 180202 (2018).
[3] G. Arregui, N.D. Lanzillotti Kimura, C. M. Sotomayor Torres, P.D. García. Anderson photon-phonon co-localization in certain random superlattices. **Phys. Rev. Lett.** 122, 043903 (2019).
[4] P.D. García, R. Bericat-Vadell, G. Arregui, D. Navarro-Urrios, M. Colombano, F. Alzina, C. M. Sotomayor-Torres. Optomechanical coupling in the Anderson-localization regime. **Physical Review B** 95 (11), 115129 (2017).

Graphene nanoarchitectures: insights from theory and experiments

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Nanostructuring graphene at the atomic scale is now possible by on-surface synthesis methods, which unite the sturdiness of covalently bonded networks with the easy tunability of molecular materials. These experimental advances have boosted the research attempts to create novel 0D, 1D and 2D carbon-based structures aimed at the development of new nanoelectronic or optoelectronic devices. However, before graphene nanostructures can be used in practical applications, an atomic level understanding and control of their properties is required. As such, *ab-initio* simulation has developed as an essential partner in the search of optimal graphene-based low dimensional materials.

In this talk, I will present some studies of graphene nanostructures, in particular graphene nanoribbons (GNRs) and nanoporous graphene (NPG), that we have perfomed in collaboration with our experimental colleagues.[1,2,3] Using density-functional theory (DFT), we have investigated their structural, electronic and transport properties, with special focus on the role of chemical doping and the creation of pores in the carbon backbone. Our findings are compared with scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoemission (ARPES) data. Depending on the conformational details and the doping mechanism, various effects are observed and explained, such as electron confinement, energy gap modification, or semiconductor-to-metal transition.

References

[1] J. Hieulle *et al.*, Nano Letters 18, 418 (2018).
[2] E. Carbonell-Sanromà *et al.*, Nano Letters 17, 50 (2017); J. Phys. Chem. C 122, 16092 (2018).
[3] Moreno *et al.*, Science 360, 199 (2018).

Figures

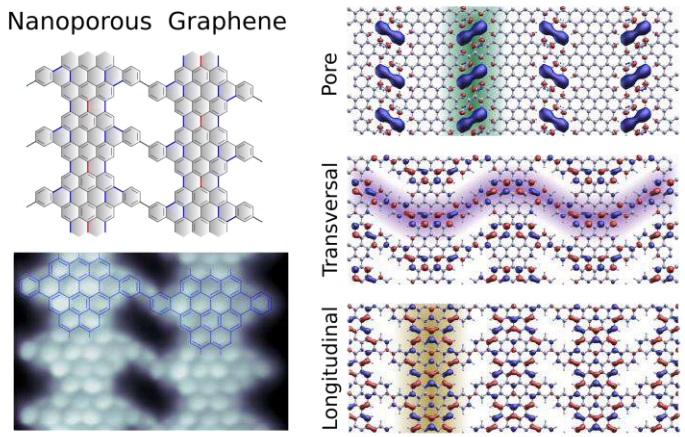

Figure 1. Left panels: schematic representation (top) and STM image (bottom) of nanoporous graphene. Right panels: DFT wave functions of pore (top), transversal (middle) and longitudinal (bands).

Single-step Modified Electrodes for Ascorbic Acid Detection in Sweat at Ultralow Potential

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We present an electrochemical sensor for the detection of ascorbic acid (AA) in sweat at ultralow potential. The sensor is based on gold electrodes modified by one-step electrodeposition of an alginate membrane where CuO nanoparticles are trapped. AA is a known reducing agent of nanostructured copper[1], and the effect is seen as a shift of the redox peaks to a positive voltage (Figure 1a). By measuring at nearly zero volts (-5 mV), the approaching of the reduction peak to this value can be detected as a growing negative current. We perform the detection of the relevant micromolar levels (Figure 1b) in neutral buffer as well as in artificial acidic sweat. The sensor does not show any cross-reactivity with typical species found in sweat such as lactic acid, glucose, urea, pyruvic acid, glutamic acid, and uric acid, showing an excellent specificity. As a nonenzymatic approach, the stability is not as compromised and the cost is reduced. Easy removal of alginate by a calcium-quelating buffer makes it possible to reuse the electrodes with a different membrane composition on-demand[2]. Finally, the sensor is fabricated on Kapton foils, an appropriate material for the construction of flexible sensors[3] that enables future integration on wearable devices for monitoring of sweat parameters and nutrient loss.

References

[1] X. Cheng et al. *Appl. Surf. Sci*. **2006**, 253, 2727–2732.
[2] A. Márquez et al. *Biosens. Bioelectron.* **2019**, 136, 38–46.
[3] D. Karnaushenko et al., *Adv. Healthc. Mater*. **2015**, 4, 1517–1525

Figure

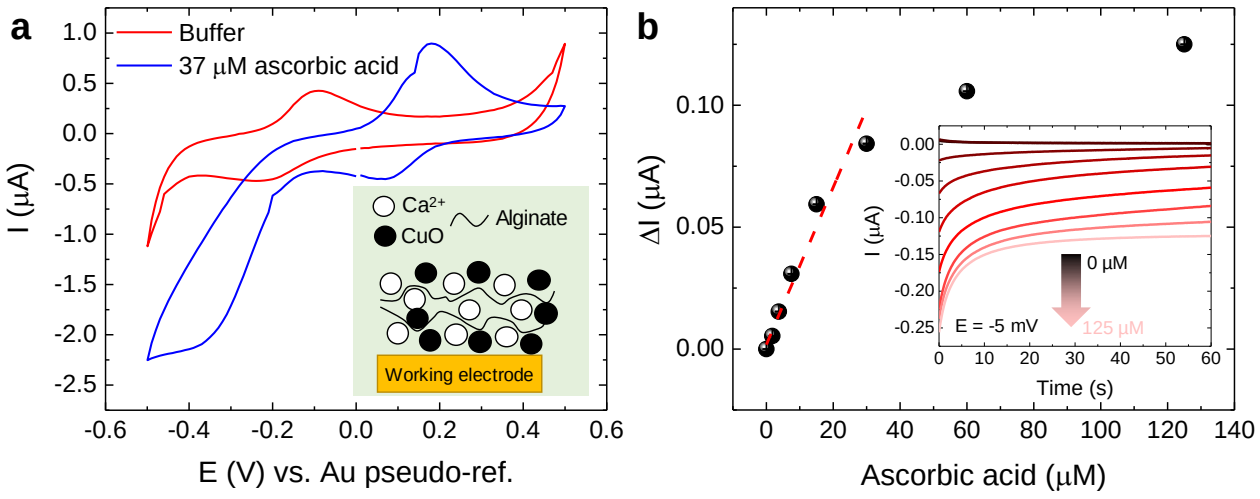

Figure 1. Ascorbic acid sensing with alginate/CuO-modified electrodes. (a) Effect of the ascorbic acid on the cyclic voltammogram of the sensor. Inset shows the composition of the membrane. (b) Calibration. Inset shows amperometric response at -5 mV.

Infrared hyperbolic metasurface based on nanostructured van der Waals materials

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Hyperbolic metasurfaces with strongly anisotropic optical properties supports deep subwavelength-scale confined surface polaritons, which present a hyperbolic dispersion [1,2]. They could extremely enhance light-matter interaction at mid-infrared and terahertz frequencies (corresponding to energies of molecular vibrations, and thermal emission and absorption) for photonic and thermal applications, such as heat management, chemical sensing and deep subwavelength imaging [2]. However, hyperbolic metasurfaces working at these frequencies have not been developed yet due to the required challenging fabrication.

In this work, we realize the first mid-infrared hyperbolic metasurface by nanostructuring a thin layer of hexagonal boron nitride —a prototypical van der Waals (vdW) polar material, which supports mid-infrared phonon polaritons with strong electromagnetic field confinement, ultraslow group velocities and long lifetimes [3,4]. We used scattering-type scanning near-field optical microscopy to directly observe phonon polaritons emerging from the hot spot at the extremity of an infrared antenna and propagating through the metasurface with in-plane hyperbolic dispersion (Figure 1), which assembles the concave (anomalous) wavefronts of a diverging polariton beam (Figure 1.C). These results show that near-field microscopy can be applied to reveal the exotic wavefronts of polaritons in anisotropic materials, and demonstrate that nanostructured vdW materials can form a highly variable and compact platform for hyperbolic infrared metasurface devices and circuits [5].

References

[1] A. V. Kildishev et al., *Science* **339**, 1232009 (2013).
[2] J. S. Gomez-Diaz, et al., *Phys. Rev. Lett,* **114**, 233901 (2015)
[3] S. Dai, et al., *Science*, **343**, 1125-1129 (2014).
[4] P. Li, et al., *Nat. Commun.* **6**, 7507 (2015).
[5] P. Li, et al., *Science*, **359**, 892–896 (2018).

Figures

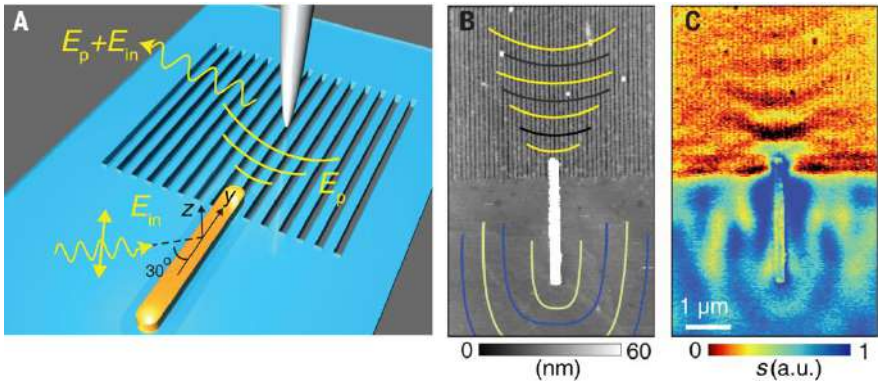

Figure 1. (A) Schematic of the experiment. (B) Topography image. The lines illustrate wavefronts of phonon polaritons on the hyperbolic metasurface (yellow and black) or phonon polaritons on the unpatterned flake (yellow and blue). (C) Near-field optical image. It clearly reveals concave wavefronts of phonon polaritons emerging from the rod's upper extremity.

Tailoring quantum confinement using extended organic nanoporous networks

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Organic nanoporous networks grown on (111) noble metal surfaces are highly successful model systems to study scattering electron phenomena. On such surfaces, the 2D molecular scaffolds are able to confine the surface state electrons and are commonly named “quantum dot arrays” [1-5]. The resulting confined states result in sizable energy shifts of the Shockley states and the formation of shallow bands, as a results from the repulsive scattering at the molecular walls and partial quantum confinement within each pore [1-5].

We have studied 6 extended 2D nanoporous networks grown on noble metal surfaces which yield single domain structures. Our findings show that depending on the geometry and building units it is possible to tune the energy shifts in opposite directions (towards and away from the Fermi energy), independently of the substrate. The nature of this effect is related to metal-organic overlayer-substrate interactions in the form of adatom-surface state hybridizations. The electronic structure in all cases is determined by two state-of-the-art, highly complementary techniques (STM and ARPES), and supported by first principles and model calculations.

References

[1] F. Klappenberger et al., Phys. Rev. Lett. 106, 026802 (2011).
[2] I. Piquero-Zulaica et al., Nature Communications 8, 787 (2017).
[3] J. Lobo-Checa et al., Science 325, 300 (2009).
[4] S. Nowakowska, et al., Small 12, 3757 (2016).
[5] I. Piquero-Zulaica et al., New Journal of Physics 21, 053004 (2019)

Figures

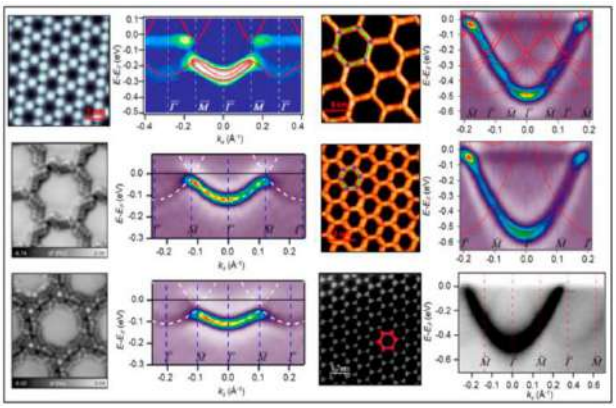

Figure 1. STM topographies and corresponding band structure of six different single domain nanoporous networks that give rise to quantum dot arrays. The fundamental energy of the bands can either shift towards the Fermi energy or away from it, even if in all cases there is evidence of electronic confinement.

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

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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. 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].

References

[1] S. Albaladejo, M. I. Marqués, M. Laroche and J. J. Sáenz, Phys. Rev. Lett. 102, 113602 (2009).
[2] V. V. Temnov, G. Armelles, U. Woggon, D. Guzatov, A. Cebollada, A. García-Martín, J. M. García-Martíın, T. Thomay, A. Leitenstorfer, and R. Bratschitsch Nat. Photonics 4, 107 (2010).
[3] S. Edelstein, R. M. Abraham-Ekeroth, P. A. Serena, J. J. Sáenz, García-Martín,and M. I. Marqués, Phys. Rev. Res. 00, 003000 (2019).

Graphene and other carbon nanoforms for a sustainable world

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Graphene and carbon nanotubes are potentially sustainable materials able to replace metals (heat and electrical transport), indium tin oxide (displays) and if not recycled, simply burned away avoiding hazardous wastes linked to metal disposal. According to IUPAC, Graphene is a single layer of hexagonally arranged carbon atoms. However, its definition gets fuzzy in research literature and even more in the industrial world.[1] It is thus quite important to fully characterize graphene and/or other carbon nanoforms in order to be able to correctly assess its performances / interest. I will describe surfactant-free, aqueous, dispersions of *single layer graphene* Eau de Graphene (EdG), in which hydroxyl ion adsorption stabilizes graphene sheets in water, [2-4] and on the associated spin-off company, Carbon Waters.[5] Information about thickness, lateral size and defect analysis of graphene in EdG will be described. Recent works on adapting the EdG strategy to carbon nanotubes will also be described.[6] Finally, starting with a nanocarbon originating from biomethane, carbon nanopucks have been thoroughly characterized and used to prepare conducting nanocarbon inks,[7] conductive rubbers,[8,9] nanocarbon/iron nanoparticle composite electrocatalysts for fuel cell technology,[10,11] and microsupercapacitors, all of them might contribute to a cleaner tomorrow.

References

[1] Segal, M. Selling Graphene by the Ton. *Nat. Nanotechnol.* **2009**, *4* (10), 612–614.
[2] Bepete, G. *et al.* Surfactant-free single-layer graphene in water. *Nat. Chem.* **9,** 347–352 (2017).
[3] Bepete, G., Pénicaud, A., Drummond, C. & Anglaret, E. Raman Signatures of Single Layer Graphene Dispersed in Degassed Water , " Eau de Graphene ". *J.phys. Chem. C* **120,** 28204–28214 (2016).
[4] Bepete, G. *et al.* "Eau de graphene" from a KC8 graphite intercalation compound prepared by a simple mixing of graphite and molten potassium. *Phys. status solidi - Rapid Res. Lett.* **10,** 895–899 (2016).
[5] Carbon waters: https://www.carbon-waters.com/.
[6] Bepete, G. et al. Hydroxide Ions Stabilize Open Carbon Nanotubes in Degassed Water, ACS Nano 2018, 12, 8606.
[7] Hof, F. *et al.* Conductive inks of graphitic nanoparticles from a sustainable carbon feedstock. *Carbon N. Y.* **111,** 142–149 (2017).
[8] Kampioti, K. *et al.* Highly Conducting, Sustainable, Nanographitic Rubber Composites. *ACS Omega* **3,** 1367–1373 (2018).
[9] ACS. From compost to composites: An eco-friendly way to improve rubber. (2018). https://www.youtube.com/watch?v=i-93J2n76Bs&feature=youtu.be
[10] Hof, F. *et al.* From Food Waste to Efficient Bifunctional Nonprecious Electrocatalyst. *Chem. - A Eur. J.* **23,** 15283–15288 (2017).
[11] Hof, F. *et al.* Graphenide solutions: A chemical platform for nanoparticle nanocarbon composites, *Chem. - A Eur. J.* 2018, 10.1002/chem.201801694

Polymerization on unconventional substrates

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In the early 1900's Fritz Ullmann first reported the synthesis of biaryls from aryl halides mediated by a fine copper powder[1], demonstrating with this the aromatic nucleophilic substitution mediated by copper, now known as Ullmann condensation reaction. More than hundred years after, this reaction is routinely used in numerous industrial applications and, nowadays it becomes widely used for the synthesis on metal surfaces of atomically precise graphene nanoribbons[2]
The next step to move toward device applications requires performing the synthesis directly on suitable substrates such as semiconducting, insulating or magnetic substrates. Whit in this context, in the present work we explore the Ullmann based synthesis of polymers on magnetic and insulating substrates. In particular we demonstrate the aryl homocoupling synthesis of 4,4-Dibromo (or diiodo)-p-terphenyl precursor into molecular poly-p-phenylene wires on the semiconductor TiO2 surface[3] and on the bimetallic (and ferromagnetic) GdAu2 surface alloy[4] . Moreover, we propose a reaction pathway during the polymerization. To monitor the chemical reaction complementary microscopic and spectroscopic surface science techniques (, scanning tunneling microscopy, X-ray photoemission spectroscopy, angle-resolved Photoemission spectroscopy) are used.

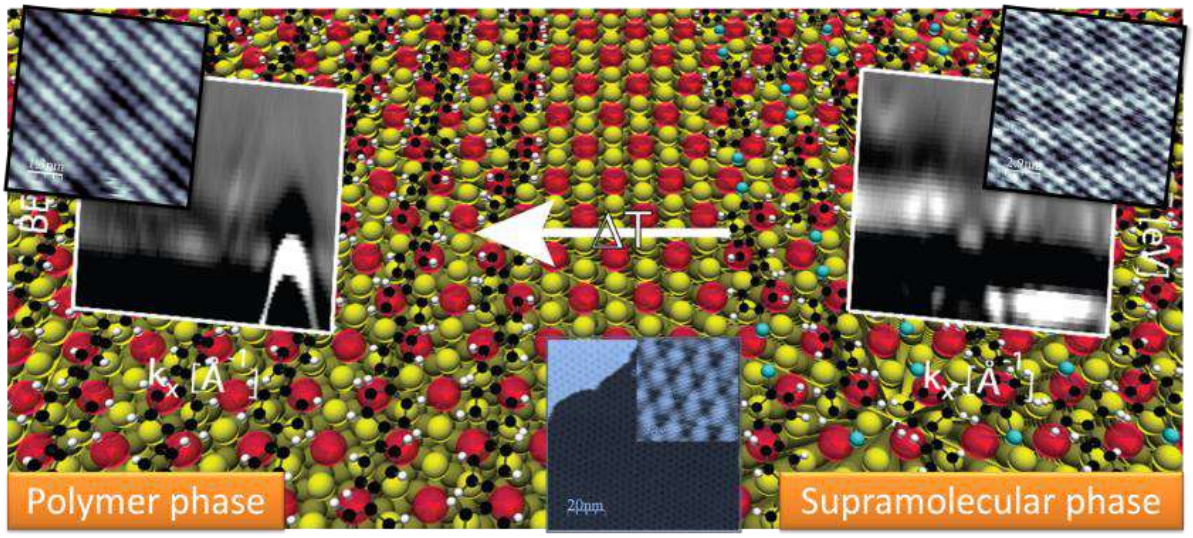

Figure 1– STM and ARPES experimental observations of Ullmann based Polymer synthesis on $GdAu_2$ alloy

References

[1] Ullmann, F. et al. Berichte der Deutschen chemischen Gesellschaft, 34, 2174 (1901); 36, 2382 (1903); 37, 853 (1904).
[2] Grill, L. et al. Nature Nanotech. 2, 687 (2007); Cai, J.; et al. Nature 466, 470 (2010); Talirz, L.; et al. Adv. Mater., 28, 6222 (2016)
(3) Vasseur, G.; et al. J. Am. Chem. Soc. 138, 5685 (2016)
(4) Abadía, M. et al. ACS Nano 11, 12392 (2017)

Composite-boson signature of atomic dimers in the interference pattern of colliding condensates

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All particles consisting of an even number of fermions are boson-like, which bears a strong consequence: they must undergo Bose-Einstein condensation.

We predict that, compared to elementary bosons, the interference pattern of two colliding BEC made of fermionic-atom dimers must have additional high frequency modes. As these new modes are many-body in essence, previous experiments performed with two rather dilute condensates have only seen interferences ruled by the condensates' momentum difference, a result obtained by taking atoms as elementary bosons. The higher frequency modes we predict result from fermion exchanges between condensates, and thus constitute a striking signature of the dimer composite nature. We analytically derive the 2-coboson spatial correlation functions and use Shiva diagrams, specific to coboson many-body effects, to identify the physical origin of these high-frequency modes and determine the conditions to see them experimentally, using optical lattices. A dimer granularity appears because Pauli blocking prevents two dimers to occupy the same site.

In the same way as the composite nature of semiconductor excitons has already revealed a breadth of remarkable effects, we anticipate cold-atom systems to provide a novel, fully controllable playground to investigate further in depth the very unique many-body effects that result from dimensionless fermion exchanges, i.e., exchange in the absence of fermion-fermion interaction. Recent optical lattices already reach densities high enough for these new many-body effects to be observable, including the signature predicted here.

References

[1] SY Siau, A. Chenu, M. Combescot, New J. Phys. 21 (2019) 043041Reference 2

Introducing Topological Quantum Chemistry and Topological Materials Data Base

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In this talk a new field that classifies all topological crystalline phases of all known materials will be introduced: Topological Quantum Chemistry (TQC). It links the chemical and symmetry structure of a given material with its topological properties. This field tabulates the data of the 10398 real-space atomic limits of materials, and solves the compatibility relations of electronic bands in momentum space. A material that is not an atomic limit or whose bands do not satisfy the compatibility relations, is a topological insulator/semimetal. We use TQC to find the topological stoichiometric non-magnetic, ``high-quality'' materials in the world. We develop several code which can compute all characters of all symmetries at all high-symmetry points in the Brillouin Zone (BZ). Using TQC we then develop codes to check which materials are topological. Out of 26938 stoichiometric materials in our filtered ICSD database, we find around 7300 topological materials. For the majority of the ``high-quality'' topological materials, we compute: the topological class, the symmetry(ies) that protects the topological class, the representations at high symmetry points and the direct gap (for insulators), and the topological index. For topological semimetals we then compute whether the system becomes a topological insulator (whose index/class we compute) upon breaking symmetries - useful for experiments. Our exhaustive results show that a large proportion of all materials in nature are topological. I will also explain an open-source code and end-user button on the Bilbao Crystallographic Server (http://www.cryst.ehu.es/cgi-bin/cryst/programs/topological.pl) which checks the topology of any material and a new materials data base (https://www.topologicalquantumchemistry.com/).

References

[1] M.G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B.A. Bernevig, Z. Wang , “A complete catalogue of High-Quality Topological Materials “, Nature 566, 480-485 (2019)

[2] B. Bradlyn, L. Elcoro, J. Cano, M.G. Vergniory, Z. Wang, C. Felser, M.I. Aroyo, B.A. Bernevig, “Topological quantum chemistry”, Nature 547 (7663), 298-305 (2017).

[3] MG Vergniory, L Elcoro, Zhijun Wang, Jennifer Cano, C Felser, MI Aroyo, B Andrei Bernevig, Barry Bradlyn, “Graph theory data for topological quantum chemistry”, Phys. Rev. E 96, 023310 (2017)

[4] Barry Bradlyn, L Elcoro, MG Vergniory, Jennifer Cano, Zhijun Wang, C Felser, MI Aroyo, B Andrei Bernevig, “Band connectivity for topological quantum chemistry: Band structures as a graph theory problem”, Physical Review B 97 (3), 035138 (2017)

[5] Jennifer Cano, Barry Bradlyn, Zhijun Wang, L Elcoro, MG Vergniory, C Felser, MI Aroyo, B Andrei Bernevig, “Building blocks of topological quantum chemistry: Elementary band representations”, Physical Review B 97 (3), 035139 (2017)

Figures

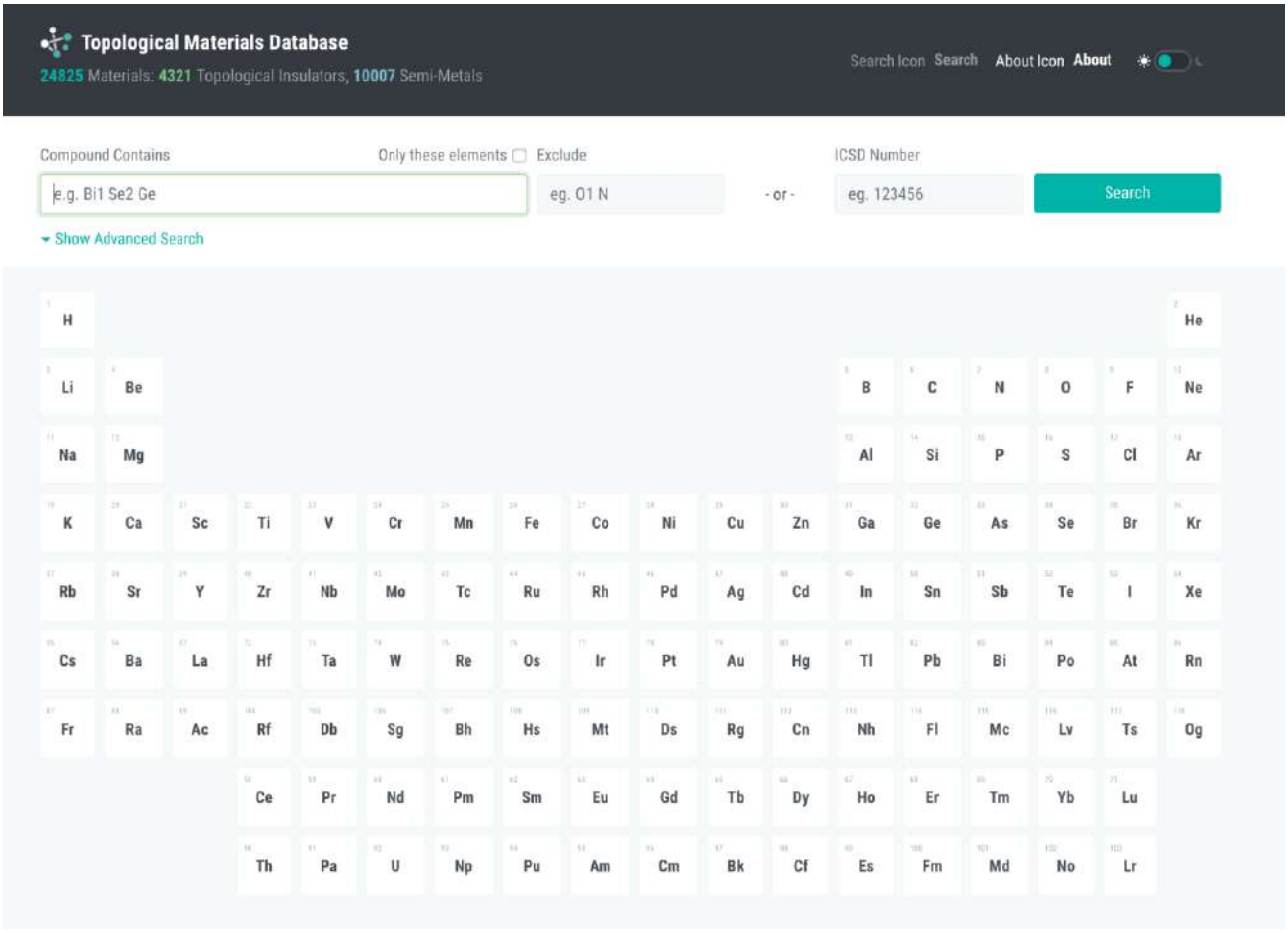

Figure 1. www.topologicalquantumchemistry.com, website for topological materials.

Graphene Integration Challenges

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Abstract

Graphene alone or in combination with other materials such as quantum dots or silicon have shown to provide enhanced performance in many applications. However, in order to integrate graphene in semiconductor devices in a cost-effective manner, it will require combining it with CMOS technology while processing the graphene into functional devices. Indeed, graphene has been monolithically integrated with CMOS technology.[1]

The fabrication of graphene at an industrial scale will require to overcome numerous challenges such as wafer scale uniformity with a high charge carrier mobility, presence of metal contamination, etc. However, wafer scale device fabrication is also critical for a successful graphene integration. At present, there is no commercial foundry able to process graphene in order to produce graphene devices (GFETs). As a consequence, we have recently launched a platform to commercialise graphene-based field effect transistor (GFETs) and thus help customers to focus on their applications rather than wasting time on graphene processing. At the same time, taking the first steps into providing a graphene commercial foundry service.

During this talk, I will cover current challenges related to wafer scale graphene growth, transfer and device fabrication.

References

[1] S. Goossens, G. Navickaite, C. Monasterio, S. Gupta, J. J. Piqueras, R. Pérez, G. Burwell, I. Nikitskiy, T. Lasanta, T. Galán1, E. Puma, A. Centeno, A. Pesquera, A. Zurutuza, G. Konstantatos and F. Koppens, Nat. Photonics 11, 366 (2017).

Figures

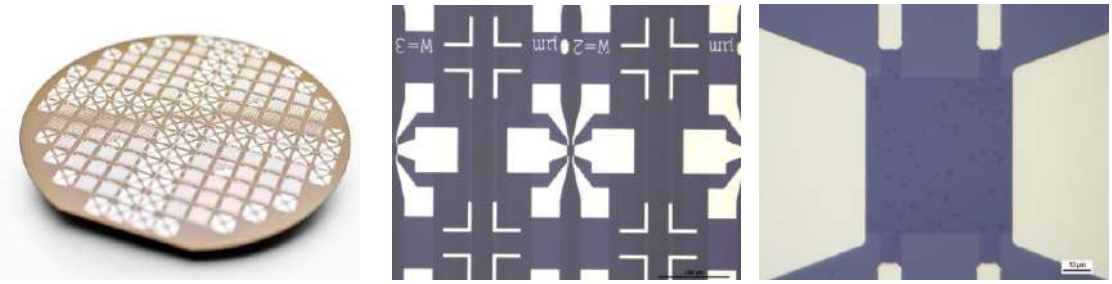

Figure 1. Wafer scale graphene field effect transistors.

ORALS
contributions

Long range topological valley currents in single layer graphene superlattice near the main Dirac point

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In topological materials, topological bands generate Hall-like conductivity and topologically protected edge states in zero magnetic field. By placing single layer graphene (SLG) on hexagonal boron nitride (h-BN), it is possible to transform SLG into a topological phase by varying their crystallographic alignment. Recent measurements of nonlocal resistances (R_{nl})[1,2] in a narrow energy range focusing with the secondary Dirac point (SDP) [3] in SLG/h-BN superlattice Hall bars have been interpreted as arising due to the valley Hall effect and quantum valley Hall state. Here we report h-BN/SLG/h-BN Hall bars which have a negligible R_{nl} of SDPs, but at the main DP R_{nl} is reaching quantum-limit at 9 K. We investigate topological valley currents near the main Dirac point and also demonstrate nonlocal measurements over a distance of 15 µm indicating ballistic behavior.

References

[1] G. Giovannetti, *et al.*, Phys. Rev. B **76**, 073103 (2007).
[2] C. R. Woods, *et al.*, Nat. Phys. **10**, 451 (2014).
[3] G. L. Yu, *et al.*, Nat. Phys. **10**, 525 (2014).

Figures

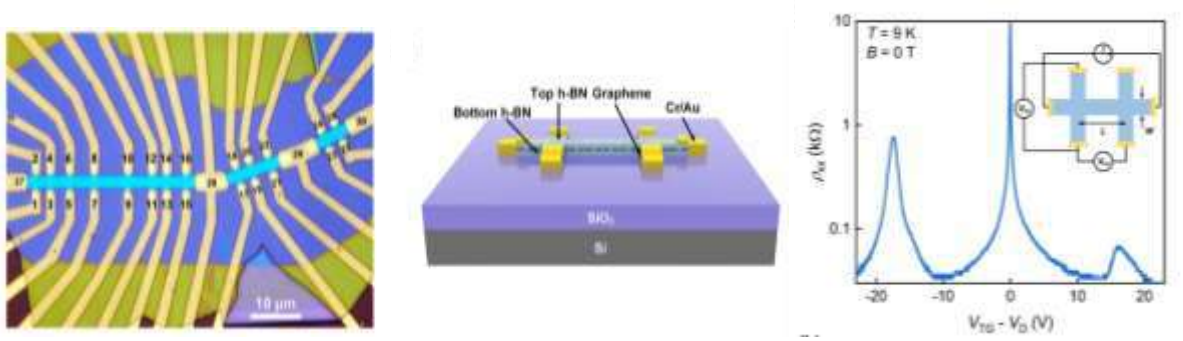

Figure 1. From left to right, h-BN/SLG/h-BN device structure via optical micrograph, schematic illustration of a typical device, Longitudinal resistivity (ρ_{xx}) *vs* gate voltage ($V_{TG} - V_D$) in zero magnetic field at 9 K. Inset shows schematic illustrations of the local measurement setup, where *L* is the distance between the current path and voltage probes, and *W* is the device width

Effect of structural disorder and chemical doping on thermal transport in Nanoporous Graphene

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Graphene nanostructures have gained increasing attention due to their great potential for applications in electronics, optoelectronics, spintronics, chemical sensing, thermoelectricity, etc. The synthesis of graphene nanostructures via top-down methods such as exfoliation and chemical reduction present well-known disadvantages such as nonregular edge structures or uncontrollable sizes. In contrast, the bottom-up organic synthesis approach has emerged as a powerful tool to design structurally well-defined nanographenes. Among them, Nanoporous Graphene (NPG) has attracted particular interest in the last years for the possibility to finely tune the structural properties of the material via the controlled manipulation of nanopores in the basal plane. The possibility to control the density and structure of the pores represents indeed a promising strategy to tune also the electrical and thermal transport in the material.
In this work, we focus on the thermal properties of NPG by studying the impact of the structural features of the material and of the chemical doping. In particular, by means of classical molecular dynamics we investigate the vibrational properties at the microscopic level. The effect of structural disorder and chemical doping on the density of states, the participation ratio, and the intrinsic character of the vibrational modes is analyzed. Finally, the contribution of each single mode to the overall thermal conductivity is calculated, highlighting the most effective vibrations responsible for heat transport in NPG.

References

[1] Moreno, César, et al. "Bottom-up synthesis of multifunctional nanoporous graphene." *Science* 360.6385 (2018): 199-203.

Figures

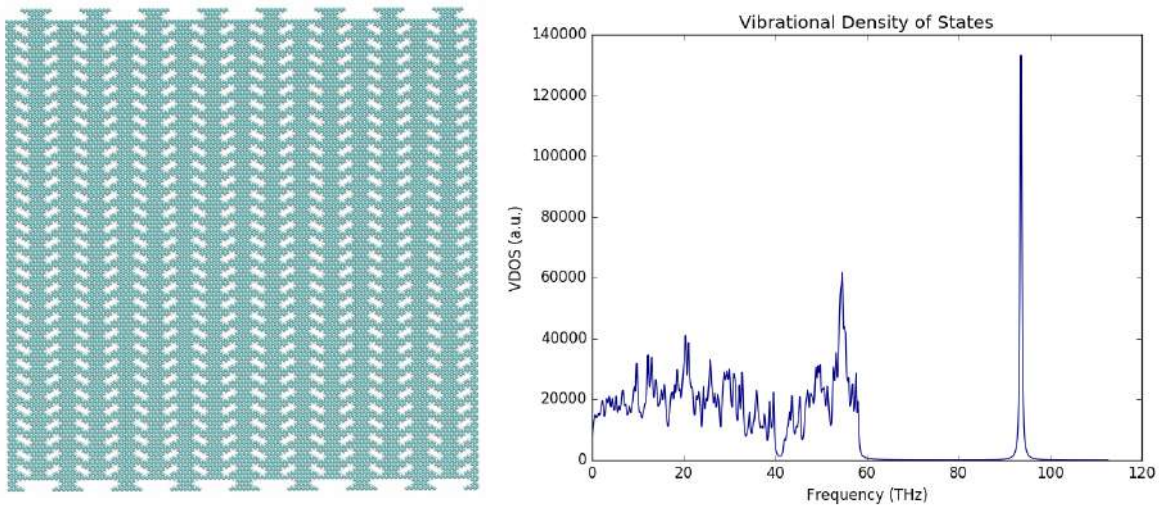

Figure 1. (Left) Nanoporous Graphene sample with 24800 atoms. (Right) Vibrational Density of states of NPG.

Large-scale simulations of soft polymeric particles at liquid-liquid interfaces: Effects of network topology on the miscibility of immiscible solvents

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As an alternative to rigid particles, soft particles have an enormous potential for emulsion stabilization. In particular, they may serve as compatibilizers of immiscible fluids [1] and have a high degree of deformability, penetrability and stimuli responsive properties. However, for exploiting them in many practical applications it is essential to obtain a (still scarce) fundamental understanding of the interfacial properties as a function of the soft particle topology and its conformations under different conditions (temperature, pH, etc). In this contribution, we employ in-silico realistic protocols for the design of nanogels, microgels [2] and globular single-chain nanoparticles [3], as examples of soft polymeric objects. We present an intensive computational study of the conformations and the effect of the internal network structure of the former particles on the mixing properties of immiscible liquids [4]. We investigate the whole range of particle's cross-linking degree and strength of the interfacial fluctuations. Comparisons are provided with respect to ideal regular network topologies (diamond-like) generally employed in the literature. In both cases, we include explicit solvent molecules and monomer-solvent excluded volume interactions. Contrary to previous studies where excluded volume was not considered [1], we find that homogeneous mixtures cannot be really formed inside the soft particle, independently of the interface strength and the network topology. Moreover, the solvent uptake is optimized for moderate cross-link densities (~20%), and more important, the specific network topology (disordered or regular) does not play a significant role on the solvents' mixing inside the particle. The implications of such findings are discussed with respect to possible experimental synthesis routes that may attempt to tune the particle's internal structure. Finally, results for the solvent dynamics inside the particle and for particle diffusion along the interface are discussed. The particle exhibits striking hopping-like diffusion, suggesting an effective activated dynamics through cooperative rearrangement of the solvents.

References

[1] R. A. Gumerov, *et al.* , ACS Macro Lett. 5, 612 (2016)
[2] A.J. Moreno, F. Lo Verso, Soft Matter 14, 7083 (2018)
[3] F. Lo Verso, J.A. Pomposo, J. Colmenero, A.J. Moreno, Soft Matter 11, 1369 (2015)
[4] D.J. Arismendi-Arrieta, A.J. Moreno, submitted (2019)

Subnanometer 2D-confinement of poly(ethylene oxide) in graphene-based materials: effect of polymer topology

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The confinement of both molecular and macromolecular systems at nanometer length scales can lead to significant changes in observables such as glass transition temperature and melting point. Graphene-based materials are exceptional hosts to study confined polymers at the subnanometric scale due to the ability to control and tune their degree of oxidation and exfoliation and, therefore, to control the strength of the interaction between host and macromolecules [1]. In fact, poly(ethylene oxide) (PEO) is able to intercalate into the interlayer space of graphite oxide (GO) and to form extremely 2D confined monolayers of about 3.3 Å with restricted mobility [2] and conformations [1, 3]. In this presentation, we will show our recent studies on the intercalation kinetics of linear and cyclic PEO into GO, in going from low molecular weight oligomers (crown ether case) to higher molecular weight polymers. In these studies we made use of the total absence of glass transition and melting of the intercalated PEO oligomers and polymers to monitor the evolution of the glass transition and melting of the non-intercalated material as a function of time. This unique property of the intercalated (and confined) phase in GO allowed us to quantify the composition of non-intercalated material. We first demonstrate that the enormous difference in the intercalation rate between cyclic and linear oligomers can be used as a method to selectively separate the cyclic molecules from the linear ones in the melt [4] or in solution [5]. Secondly, these differences in the intercalation rate become smaller with increasing molecular weight. By introducing fixed pillars into the GO structure that operate as physical barriers against the polymer diffusion, we demonstrate that it is possible to restrict the intercalation of cyclic PEO into graphite oxide, whilst allowing the linear analog to diffuse through the graphite oxide layers (Figure 1). This important finding could be the basis for developing a method of purification of cyclic polymers.

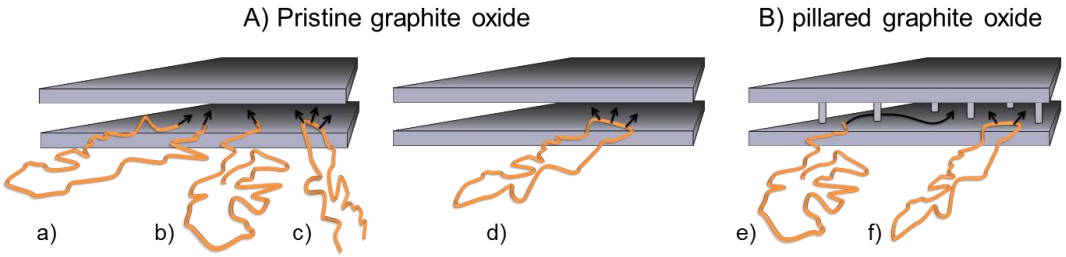

Figure 1. Melt intercalation of PEO into (A) pristine GO and (B) pillared GO. (a, b) Intercalation of linear chains driven by end-group diffusion and (c) main-chain diffusion (c). (d) Intercalation of cyclic PEO into GO driven only by main-chain diffusion. Intercalation of (e) linear and (f) cyclic PEO into a pillared GO, where it is predicted that intercalation of a linear chain is favored respect to that of a cyclic chain.

References

[1] F. Barroso-Bujans, F. Fernandez-Alonso, J.A. Pomposo, S. Cerveny, A. Alegría, J. Colmenero, ACS Macro Lett., 1 (2012) 550
[2] F. Barroso-Bujans, S. Cerveny, Á. Alegría, J. Colmenero, Macromolecules, 46 (2013) 7932
[3] F. Barroso-Bujans, F. Fernández-Alonso, S. Cerveny, S. Arrese-Igor, Á. Alegría, J. Colmenero, Macromolecules, 45 (2012) 3137
[4] F. Barroso-Bujans, A. Alegria, Phys. Chem. Chem. Phys., 19 (2017) 18366
[5] D. Ruiz, A. Alegria, F. Barroso-Bujans, Sep. Purif. Technol., 213 (2019) 142

What will stop the exfoliation of MoS_2

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The liquid-phase exfoliation (LPE) is a technique with the potential for large scale production of 2D materials [1]. One of the promising 2D materials for applications in electronics, sensors, Li-ion batteries, and others is MoS_2 [2]. In our contribution, we will present a limitation of the conventional LPE process. The oxidation depends on the initial concentration of MoS_2 powder and the type of solution, in which the powder is dispersed. If the initial concentration of the MoS_2 powder exceeds the critical value of approximately 12 mg/ml, the oxidation of MoS_2 towards MoO_x nanoparticles occurs (Figure 1). In our presentation, we will discuss the fundamental limitation of the LPE process and analyze the generated MoO_x nanoparticles.

Acknowledgments

We acknowledge the financial support of the APVV-15-0641 project.

References

[1] Tao, H. et al. Scalable exfoliation and dispersion of two-dimensional materials-an update. Phys. Chem. Chem. Phys. 19, 921–960 (2017).
[2] Gupta, A., Sakthivel, T. & Seal, S. Recent development in 2D materials beyond graphene. Prog. Mater. Sci. 73, 44–126 (2015).

Figures

Figure 1. The MoO_x nanoparticles produced from 60 mg/ml of MoS_2 in (from left) NMP, water, 45% ethanol in water.

Multi-probe scanning tunneling spectroscopy for in-plane electronic transport: theory and experiment

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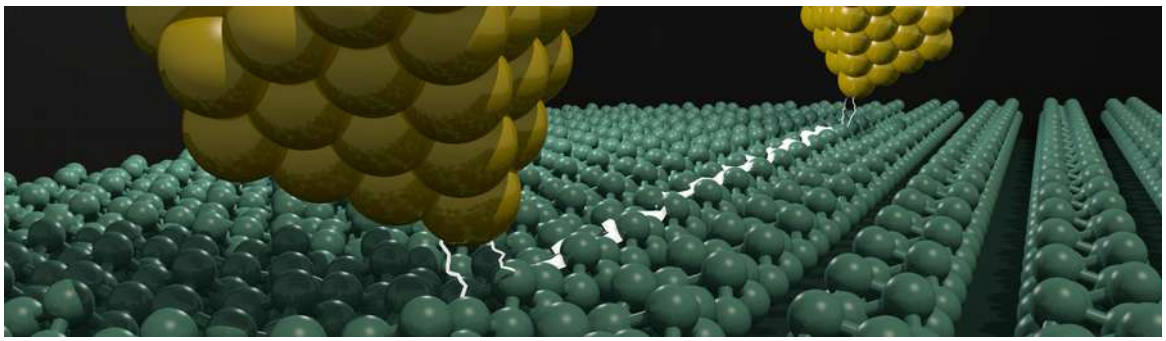
In a typical experiment using a Scanning Tunneling Microscope (STM) for spectroscopy one measures the electronic transport from the STM tip to the bulk substrate, having an adsorbed molecule or the substrate surface itself as an intermediary which is intended to be characterized. However, the determination of intrinsic transport properties from low dimensional systems (1-D or 2-D) requires at least two in-plane contacts, whose fabrication at nanoscale with high precision can be very challenging. Another possibility is the use of multi-probe STM where more than one tip approach simultaneously the system under analysis with atomic precision.

We introduce a methodology for the characterization of the in-plane electronic transport in atomic-scale circuits engineered on surface with a two-probe STM/spectroscopy.[1] In this joint theoretical and experimental work, we take as a proof of concept the anisotropic Germanium (001) surface and demonstrate a quasi-one-dimensional coherent transport of hot electrons through the Germanium dimers in the surface. Realistic first-principles calculations using Density Functional Theory together with Non-Equilibrium Green's Function formalism [2, 3] of a four-terminal setup involving up to 5000 atoms were carried out to simulate the two-tip experiment on the semiconductor surface. Comparison of both experimental and theoretical results confirm a quasi-ballistic coherent electronic transport through unoccupied states of Germanium dimer wires on the surface.

References

[1] M. Kolmer, P. Brandimarte *et al*. Nature Comm. **10**, 1573 (2019).
[2] E. Artacho *et al*. Phys. Stat. Sol. (b) **215**, 809 (1999); J. M. Soler *et al*. J. Phys.: Cond. Mat. **14**, 2745 (2002).
[3] M. Brandbyge *et al*. Phys. Rev. B **65**, 165401 (2002); N. Papior *et al*. Comp. Phys. Comm. **212**, 8 (2017).

Figures



Exciton Coupled to Fermi-Sea Polarizations In Semiconductor Quantum Wells and Transition-Metal Dichalcogenides

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Optical spectra associated with excitons in the presence of a Fermi sea (FS) in bulk or semiconductor quantum wells have been a subject of great interest for decades. Depending on the doping concentration, the Coulomb interaction between the photocreated exciton and the FS electrons can lead to various exotic complexes that come from the dressing of the exciton by Fermi-sea excitations, in the form of FS electron-hole pairs. At low doping, a bound state can emerge from the interaction of a trion and a FS hole, known as Suris tetron. [1,2] When the FS contains just one electron, this 4-particle complex reduces to the conventional X^- trion because there is no other hole state for the FS hole to scatter into to possibly form a bound state with the trion through repeated interactions.

Recently, we have developed a theory to study the exciton and its interaction with doped electrons in semiconductor quantum wells and found an interesting cross-over behavior of trion-hole complex and exciton polaron[3]. We show that an exciton-single-pair complex can exist by only keeping single electron-hole pair excitations in the Fermi sea. This 4-body complex behaves like a Fermi-sea hole weakly bound to a trion for $k_F\, a_x << 1$, where k_F is the Fermi wave-vector and a_x the exciton Bohr radius. The oscillator strength of photo-absorption associated with this trion-hole bound state increases as k_F increases. As k_F continues to increase, the feature of trion-hole bound state becomes unrecognizable, while the exciton state dressed by scattered electron-hole pairs (which can be interpreted as an exciton-polaron) becomes more pronounced. The evolution of the excitation spectra of these 4-particle coupled states (one exciton and one Fermi-sea electron-hole pair) as k_F increases reveals the cross-over from trion-hole resonance to exciton-polaron resonance, which is associated with the internal reconfiguration of the 4-body complex in the presence of the Fermi sea.

The same theoretical formalism has been extended to double quantum wells under electric field and to monolayer transition-metal dichalgogenides (TMDs) with the addition of spin-valley effects and suitable quasi-2D dielectric screening . The comparison of our theretical predictions with available experimental data (including reflance and photoluminecence pectra) will be presented.

References

[1] R. A. Suris, V.P. Kochereshko, G.V. Astakhov, D.R. Yakovlev, W. Ossau, J. Nurnberger, W. Faschinger, G. Landwehr, T. Wojtowicz, G. Karczewski, and J. Kossut, Phys. Stat. Sol. (b) 227(2), 343, (2001).
[2] A. V. Koudinov, C. Kehl, A. V. Rodina, J. Geurts, D. Wolverson, and G. Karczewski, Phys. Rev. Lett. 112, 147402 (2014).
[3] Y. C. Chang, S. Shiau, M. Combescot, Phys. Rev. B **98**, 235203 (2018)

Orientation dependent Cu oxidation and anomalous Raman shift for the graphene-copper system

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The interplay between graphene and its supporting substrate plays a key role in the performance of any graphene-based device, and therefore a detailed understanding of the graphene-substrate interaction is of paramount importance for any devised application. Due to the good tradeoff between manufacturing cost and quality of CVD graphene grown on polycrystalline Cu foils, this system is one of the most widely used in the industry. However, a detailed knowledge of the influence of Cu grain orientation on graphene properties and vice versa is still lacking. In this work the oxidation resistance of graphene covered Cu have been investigated as a function of Cu grain orientation, as well as the Raman properties of the obtained graphene monolayer [1]. Our results show that while (100) and (111) Cu grains behave according the well-known graphene-enhanced oxidation [2,3], (110) grains present a superior oxidation resistance compared to uncovered Cu (Figure 1), and an anomalous shift of its graphene 2D Raman band (Figure 2). This shift cannot be explained by the known effects of strain and doping [4]. These results are interpreted in terms of a weak graphene-Cu coupling at the (110) grains, and show that graphene can actually be used as anticorrosion coating, contrary to previously reported. The anomalous shift is suggested to be the result of an enhanced outer Raman scattering process which surpasses the usually dominant inner process [5]. Since Raman spectroscopy is widely used as first and main characterization tool of graphene, the existence of an anomalous shift on its 2D band is interesting not only for the theory of Raman scattering and more importantly, but also may have profound implications from an experimental point of view.

References

[1] J. Bartolomé, L. Álvarez-Fraga, M. X. Aguilar-Pujol, S. Cortijo, A. Cremades, C. Prieto and A. de Andrés, *2D Mater.* **6,** 015023 (2019).

[2] F. Zhou, Z. Li, G. J. Shenoy, L. Li and H. Liu, *ACS Nano*, 7, 6939–6947 (2013).

[3] L. Álvarez-Fraga, J. Rubio-Zuazo, F. Jiménez-Villacorta, E. Climent-Pascual, R. Ramírez-Jiménez, C. Prieto and A. de Andrés, *Chem. Mater.* **29,** 3257 (2017).

[4] J. E. Lee, G. Ahn, J. Shim, Y. S. Lee and S. Ryu, *Nat. Commun.*, **3**, 1024 (2012).

[5] S. Berciaud, X. Li, H. Htoon, L. E. Brus, S. K. Doorn and T. F. Heinz, *Nano Lett*. **13**, 3517 – 3523 (2013).

Figures

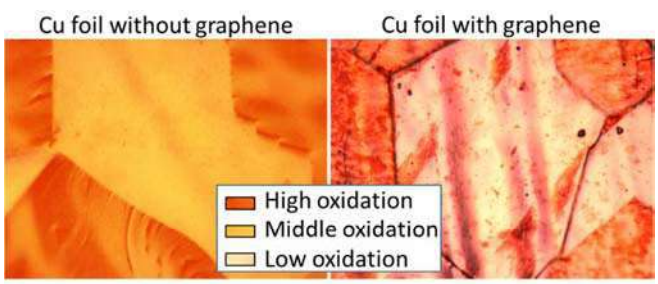

Figure 1. Oxidation of Cu foil with and without graphene for different grain orientations.

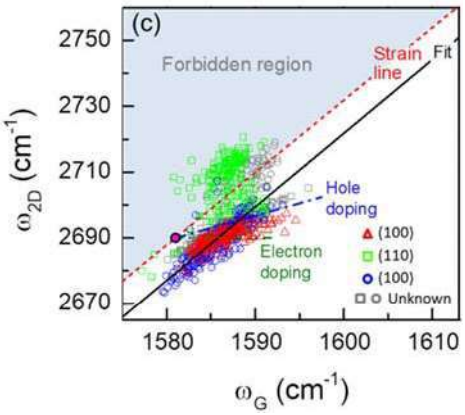

Figure 2. Raman 2D peak position versus G peak position of graphene as a function of Cu grain orientation.

Nanoclays for industrial decontamination applications

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Abstract

Removal of emerging contaminants is one of the most significant and difficult environmental problems to treat since many of these substances are of synthetic origin and a complex molecular structure, making them more stable and difficult to biodegrade. Drinking water is an increasingly scarce commodity, especially in the countries with the lowest human development index, where millions of people do not have any access to sources of clean water to meet their basic needs and often becomes vehicle diseases. That is why water pollution is an issue of vital importance to be solved. Sorption techniques produce high quality treated effluent and sorption processes have been investigated as a method of removing emerging contaminants wastewater. Our work has been to study the adsorption of different emerging contaminants from pharmaceutical and food industries by nanoclays, both natural and modifed ones. Results show a strong interaction between clays and the emerging contaminants because of the Van der Waals bonds between the organic substances and the adsorbent when the adsorption takes place.

References

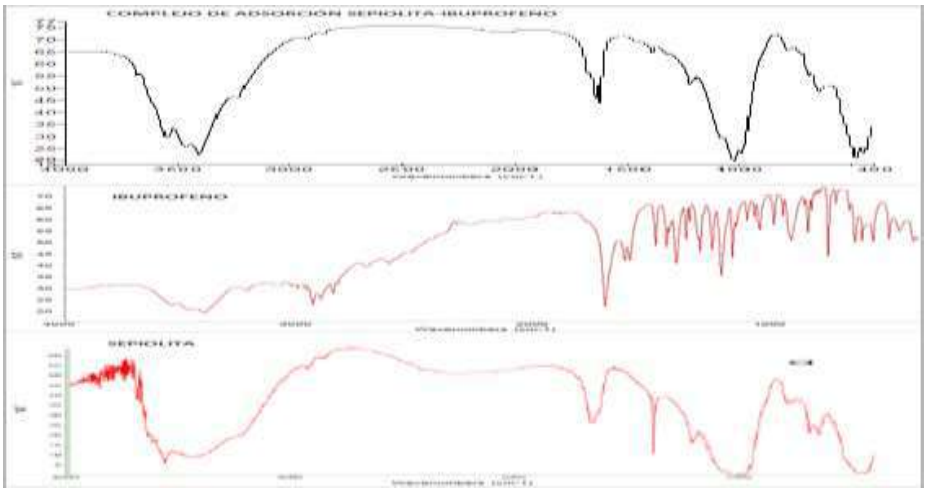
[1] C. del Hoyo Martínez, J. Cuéllar Antequera, V. Sánchez Escribano, M. S. Lozano García, R. Cutillas Díez, " Clays and Clay minerals and their environmental application in Food Technology", Geophysical Research Abstract. EGU. Vol 15, 13726-13728. 2013.

[2] C. del Hoyo Martínez, M. S. Lozano García, V. Sánchez Escribano, J. Cuéllar Antequera, "Modified Nanoclays for an Environmental Application". Phantoms Foundation Imagenano Vol. 3, 8-10. 2015.

[3] Lozano García, M. S. "Study of nanoclays adsorbents for a sustainable application". PhD Thesis. University of Salamanca. 2016.

[4] M. S. Lozano García, C. del Hoyo Martínez, J. Cuéllar Antequera V. Sánchez Escribano, "Technique for adsorption of contaminants by nano clays". Phantoms Foundation Imagenano Vol. 3, 17-19. 2015.

Figures



Cryo-etching method for quantum constrictions in encapsulated graphene

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Abstract

We report on a novel implementation of the cryo-etching method, which enabled us to fabricate very low roughness hBN-encapsulated graphene nanoconstrictions with unprecedented control of the structure edges; the typical edge roughness is on the order of a few nanometers. We characterized the system by atomic force microscopy and used the measured parameters of the edge geometry in numerical simulations of the system conductance, which agree quantitatively with our low temperature transport measurements. The quality of our devices is confirmed by the observation of well-defined quantized $2e^2/h$ conductance steps at zero magnetic field. To the best of our knowledge, till now, this observation is the clearest quantization in physically etched graphene nanoconstrictions.
The proposed cryo-etching method is also scalable; we argue therefore that the success in the fabrication of such high quality simple systems and the scalability of the technique opens a novel promising possibility of producing more complex truly-ballistic devices based on graphene.

References

[1] B.Terres et al., Nat. Commun., 7, 11528 (2016)
[2] J.M.Caridad et al., Nat.Commun., 9, 659 (2018)
[3] V.Clericò et al., Phys.Status Solidi A, 215 1701065 (2018)
[4] V.Clericò et al., https://arxiv.org/abs/1902.07459

Figures

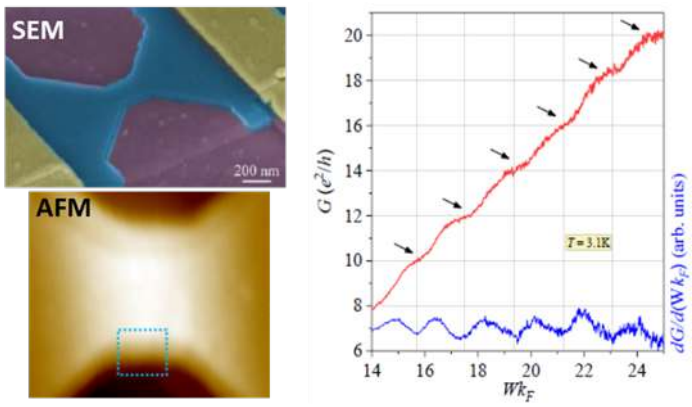

Figure 1. Top left: Coloured tilted SEM image of encapsulated grapheneNC.
Bottom left: AFM mage of encapsulated graphene NC. Right: Conductance G (red line) and transconductance (dG/dWk_F) versus Wk_F, where W is the width of the NC and k_F is the Fermi wavenumber. Black arrows highlight the position of the plateaus of conductance G separated by $2e^2/h$.

Quantum transport in van der Waals heterostructures at room temperature

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Interfacial charge transfers and Coulomb interaction at the semiconductor heterostructures give rise to emergent phenomena, which are attractive for both fundamental and applied physics [1, 2]. In conventional epitaxially grown heterostructures, mostly based on III-V semiconductors, the Coulomb interaction of charge carriers is typically weak due to small exciton binding energy and strong screening effects. These conditions render a weak interlayer charge coupling even though the interface in this structure is clean and abrupt. As a result, the quantum phenomena were usually observed at cryogenic temperature, which severely limits their novel physics for pragmatic applications. Van der Waals heterostructures, which consist of two-dimensional layered materials components, have been emerging as promising candidates for studying quantum phenomena at high temperature owing to their strong Coulomb interaction and weak screening effects. The exciton binding energy in these heterostructures has been reported in the range of hundreds of meV, allowing to observing various quantum phenomena at much higher temperature, and even at room temperature [3]. In this presentation, we report observation of the room-temperature quantum interference and Coulomb drag in the multilayer WSe_2 transistor *via* graphene contacts to its top and bottom layers separately. Central layers of WSe_2 act as an insulating region with few-nanometer width, which separate the top and bottom conducting channels spatially and provide a strong Coulomb interaction between them, leading to observing large conductance oscillations at room temperature [4]. The gradual suppression of the oscillations with increasing applied magnetic field and/or injected current further confirms the quantum interference phenomenon. As the temperature decreases, the Coulomb drag effect is obviously represented in the system due to the extended thickness of the insulating region. We also report spin transports in these heterostructures at room temperature under external magnetic field. Our results open up a new opportunity for realization of advanced quantum electronics and spintronics operating at high temperature.

References

[1] H. Kroemer, Nobel Lecture: Quasielectric fileds and band offsets: Teaching electrons new tricks, Rev. Mod. Phys. 73 (2001) 783.
[2] A. Soumyanarayana *et al*., Emerging phenomena induced by spin-orbit coupling at surface and interface, Nature 539 (2016) 509.
[3] M.-H. Doan *et al*., Charge transport in MoS_2/WSe_2 van der Waals heterostructure with tunable inversion layer, ACS Nano 11 (2017) 3832.
[4] M-H. Doan *et al*., Room-temperature mesoscopic fluctuations and Coulomb drag in multilayer WSe_2, Adv. Mater. 31 (2019) 1900154.

Engineering of Magnetic Nanotubes Based on Nanoporous Anodic Alumina

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Magnetic nanoparticles are widely used in biomedical applications due to their nanometric size, properties, and versatility. The applications of magnetic nanoparticles in biomedicine are categorized into analytical and therapeutic applications. Analytically, magnetic nanoparticles are used as magnetic carriers in separation processes, biosensors for the detection of molecular recognition events, and as contrast agents for magnetic resonance imaging [1]. The main therapeutic uses are magnetic drug delivery (can be used to improve chemotherapy in cancer treatment delivering bioactive compounds into cells) and hyperthermia during cancer therapy where the local heating of tumor cells can be achieved by inserting magnetic nanoparticles and exposing them to AC fields [2].

In this work we present hollow magnetic nanotubes based on nanoporous anodic alumina. They are obtained by pulse electrochemical anodization performed in galvanostatic conditions (Fig. 1) [3,4]. Fabricated nanotubes present low size dispersity and their length can be tuned adjusting pulse anodization parameters. They become magnetic by the attachment of a reduced quantity of ferric nanoparticles (Fig. 2). The surface of the nanotubes can be conveniently functionalize to bind to specific biomolecules and the inner part of the nanotube can be used as a nanocontainer for the drugs to be locally delivered.

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References

[1] S. Maher, A. Santos, L. Wang, T. Kumeria, et al. J. Mater. Chem. B, 5, 4097 (2017).
[2] G. Rajeev, A.J. Cowin, N.H. Voelcker, and B. Prieto Simon, Front. Chem. 7, 438 (2019)
[3] E. Xifre-Perez, J. Ferre-Borrull, J. Pallares, L. F. Marsal, Micropor Mesopor Mat. 239, 363 (2017).
[4] A. Santos, G. Macias, J. Ferré-Borrull, J. Pallarès, L.F. Marsal, ACS Appl. Mater. Interfaces, 4, 3584 (2012).

Figures

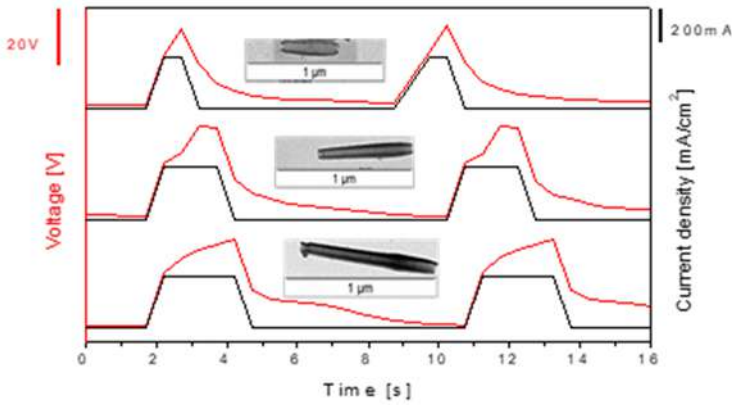

Figure 1. Current/voltage over time characteristic for galvanostatic pulse anodization.

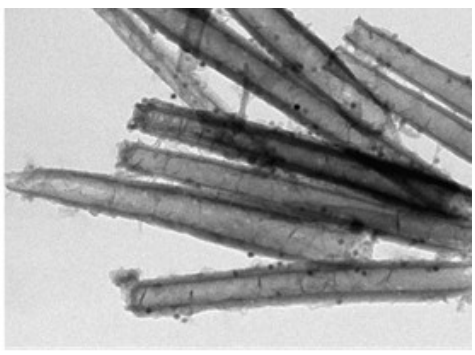

Figure 2. TEM image the anodic alumina nanotubes with magnetic nanoparticles attached.

Electron beam splitting and interferometry with graphene nanoribbons

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In this talk I will describe our recent advances in understanding graphene nanoribbons (GNRs) as interesting building blocks for constructing electron quantum optics circuitry. We have previously shown by atomistic simulations that two crossed GNRs under suitable conditions can operate as an electron beam splitter [1]. Here we extend this work and combine this basic device to form more complex electronic networks. One example is a Mach-Zehnder type interferometer and we determine the impact of a perpendicular magnetic field on its electronic transport properties.

References

[1] P. Brandimarte, M. Engelund, N. Papior, A. Garcia-Lekue, T. Frederiksen, D. Sánchez-Portal, *A tunable electronic beam splitter realized with crossed graphene nanoribbons*, J. Chem. Phys. 146, 092318 (2017)

Figures

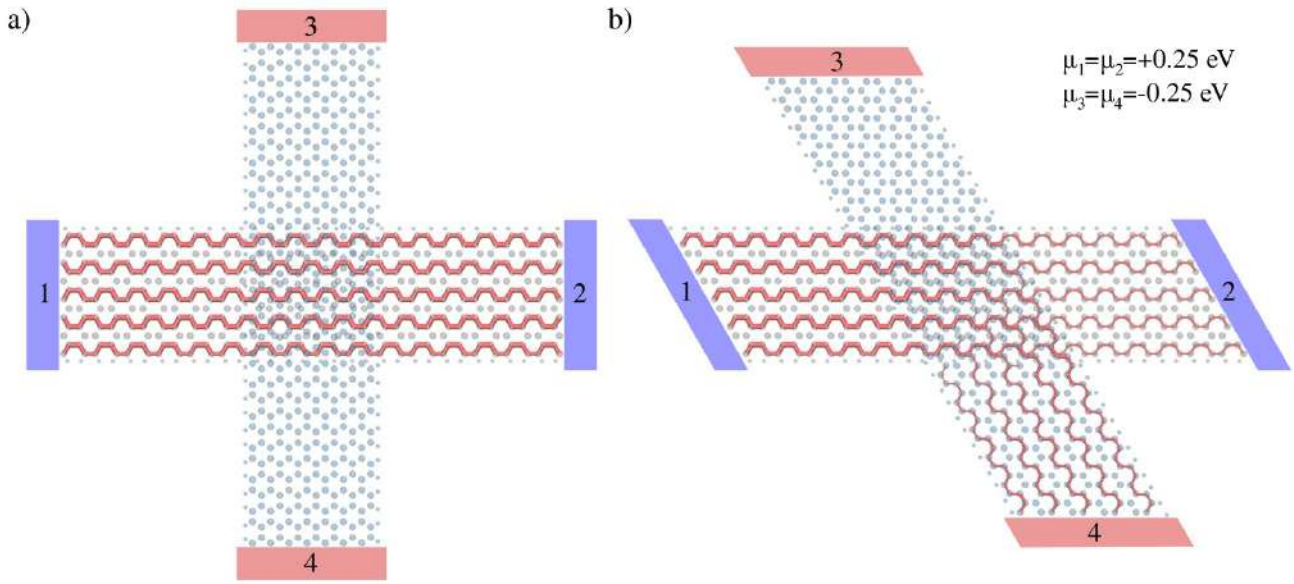

Figure 1. Electron beam splitting in devices of two crossed GNRs separated by a van der Waals-distance of ~3.3 Å. (a) In a 90 degree crossing, electrons injected from electrode 1 are mostly transmitted to electrode 2. (b) In a 60 degree intersection, the incoming electron from electrode 1 can be split with a near 50-50 probability into the outgoing electrodes 2 and 4, in analogy with an optical beam splitter. Adapted from Ref. [1].

Kinetic modeling of nanocomposites formation during co-deposition of binary films

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Abstract

The processes occurring during a thin film growth of two immiscible components are investigated by using proposed mathematical models [1, 2]. The proposed model is based on rate equations and includes the processes of adsorption, phase separation, surface segregation, surface and bulk diffusion. The mathematical descriptions of the processes of phase separation and surface segregation are based on the Cahn Hilliard equation and Gibbsian segregation model, respectively. The numerical calculations revealed that the growth rate, diffusion coefficient near the surface D_0, the concentrations of thin film constituents, the solubilities of thin film components were the important factors determining the phase structure of the thin films. Moreover, the numerical results showed that the phase structure was related to the ratio of diffusion coefficient near the surface over the growth rate D_0/V_{ad}. The binary thin films tended to grow in a columnar manner when either the relatively high values of D_0/V_{ad} or the relatively low differences between the contents of both film constituents were used. The surface diffusion dominated during the growth of the columnar structures. The change from a columnar pattern to one containing globular nanoparticles could be achieved either by decreasing the value of $D_0/V_{ad,}$ or by increasing the difference between the contents of the film components. The bulk diffusion was responsible for the formation of globular nanoparticles embedded in another phase. Same transition from a columnar pattern to one containing globular nanoparticles resulted from the increase in solubilities of both components. The influence of the surface segregation on the phase structure during a thin film growth was also analyzed. These modeling results were compared to the experimental data taken from literature where the C:Ni thin films were grown at different contents of Ni and substrate temperatures. The conclusions about the growth mechanisms of the thin films were drawn. This project has received funding from European Regional Development Fund (project No 01.2.2-LMT-K-718-01-0071) under grant agreement with the Research Council of Lithuania (LMTLT) .

References

[1] G. Kairaitis, A. Galdikas, Phase separation during thin film deposition, Computional Material Science, 91 (2014) 68–74.
[2] G. Kairaitis, A. Grigaliūnas, A. Baginskas, A. Galdikas, Kinetic modeling of phase separation and surface segregation in growing a-C:Ni thin films, Surface Coatings and Technology, 352 (2018) 120–127.

Figures

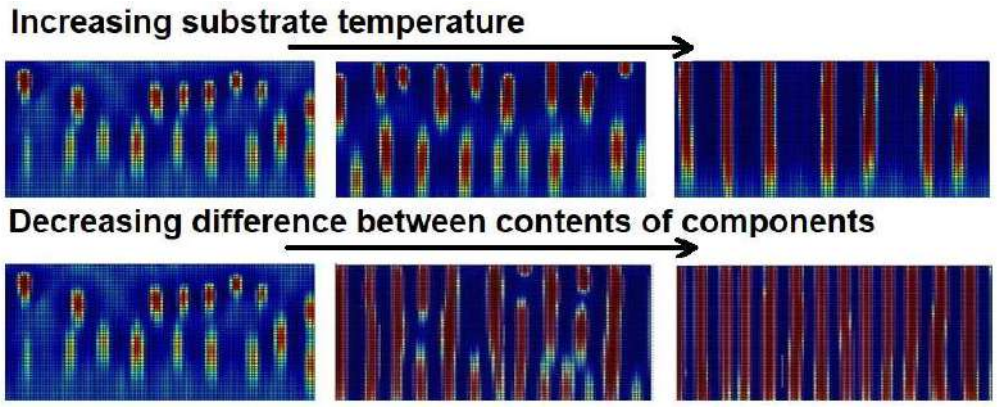

Figure 1. Influence of substrate temperature and thin film composition on phase structure

Optomechanical biosensors

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The field of Optomechanics has made impressive advances in the last decades, covering a broad range of applications going from ultrasensitive sensing to fundamental quantum studies. Particularly, the use of optomechanical devices for biosensing has acquired crescent interest in the last years. Optomechanics effects provide extraordinary sensitivity to motion, allowing the detection of mechanical modes of micro and nanostructures at very high frequencies, surpassing the GHz range. A very promising optomechanical platform for biosensing applications are semiconductor microdisks. These devices support a family of modes, the radial breathing modes (RBM), which present extremely high mechanical frequencies (> GHz) and low energy losses in liquids. These assets, together with their remarkably low masses (in the pg range), provide them with extremely low mass sensitivities and high speed, notably, while immersed in liquid [1]. In addition, semiconductor microdisks can be integrated in collective configurations, thus, improving their sensing efficiency while keeping their individual capabilities [2].

Here we show the first application of optomechanical devices as biological sensors. We have applied different individual and collective configurations of semiconductor microdisks (Fig. 1.a). We have developed a novel deposition method which allow us to precisely locate individual and alive bacteria in our sensors (Fig. 1.b). By detecting changes in their mechanical and optical modes, microdisks are capable of determining the mechanical and optical properties of *Staphylococcus Epidermidis* bacteria (Fig. 1.c).

References

[1] Gil-Santos, E. et al. High-frequency nano-optomechanical disk resonators in liquids. Nature Nanotechnology, 2015. 10, p. 810-817.
[2] Gil-Santos, E. et al. Light-mediated cascaded locking of multiple nano-optomechanical oscillators. Physical Review Letters, 2017. 118, p. 063605.

Figures

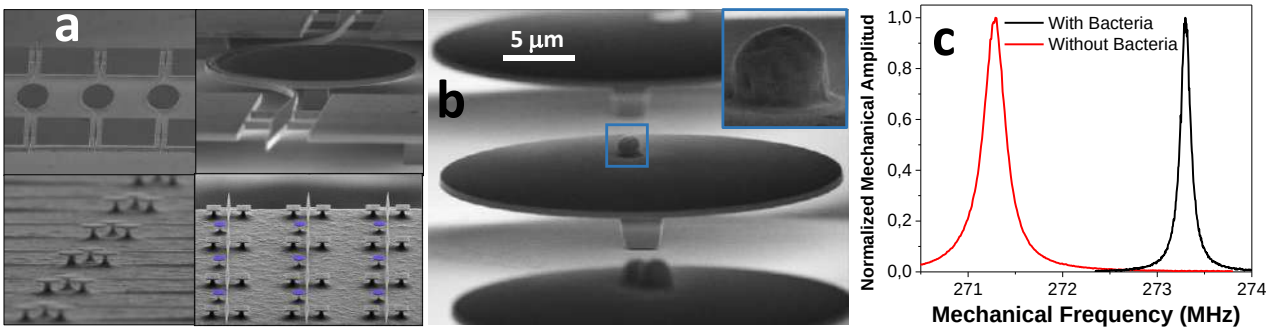

Figure 1. a. Scanning electron microscopy (SEM) images of some of the microdisks sensors configurations tested. **b.** SEM images of optomechanical microdisks (R*T=10*0.32 ⍰m2) with Staphylococus Epidermis bacteria absorbed on them. **c.** Mechanical spectra showing the first RBM resonance of a microdisk (R=5 µm and T=320 nm) without and with a Staphyloccoccus epidermis bacteria adsorbed on it.

High Performance of Electrochromic Devices based on WO3 Nanowalls

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Abstract

Tungsten trioxide thin films have been extensively studied because of their potential application in electrochromic devices. The optical properties of these films can be changed in a reversible and persistent way under the influence of an applied voltage. Electrochromism refers to the reversible change of color of thin films due to a small change in the voltage. This is important for smart windows and display applications.

Tungsten Oxide (WO_3) is a transition metal oxide with wide range of applications from gas sensors to electrochromic devices (ECD). It is difficult to prepare nanostructured materials with sputtering method in which we developed a simple method to produce WO3 nano-structures by RF magnetron sputtering. WO3 nano-walls prepared on 20 Ohm/square sputtered ITO thin films. ITO/WO3/1 M LiClO4/PC Electrolyte/ITO type ECD were prepared. ECD based on three different thicknesses of WO_3 were prepared. Performance of the ECD devices were measured by transmittance measurements applying the +-3.2 V voltage to the devices. In general, it has been observed that the turn on/off time of the devices are a few seconds. The thickest, 600 nm, WO_3 device has shown % 66.7 optical transmittance change at 700 nm within 40 s at coloration, while the medium thickness (300nm) and thinner one (180nm) has shown %54 and %32 transmittance change, respectively. Also, gaso-chromic performances of the devices were also reviewed.

Figure

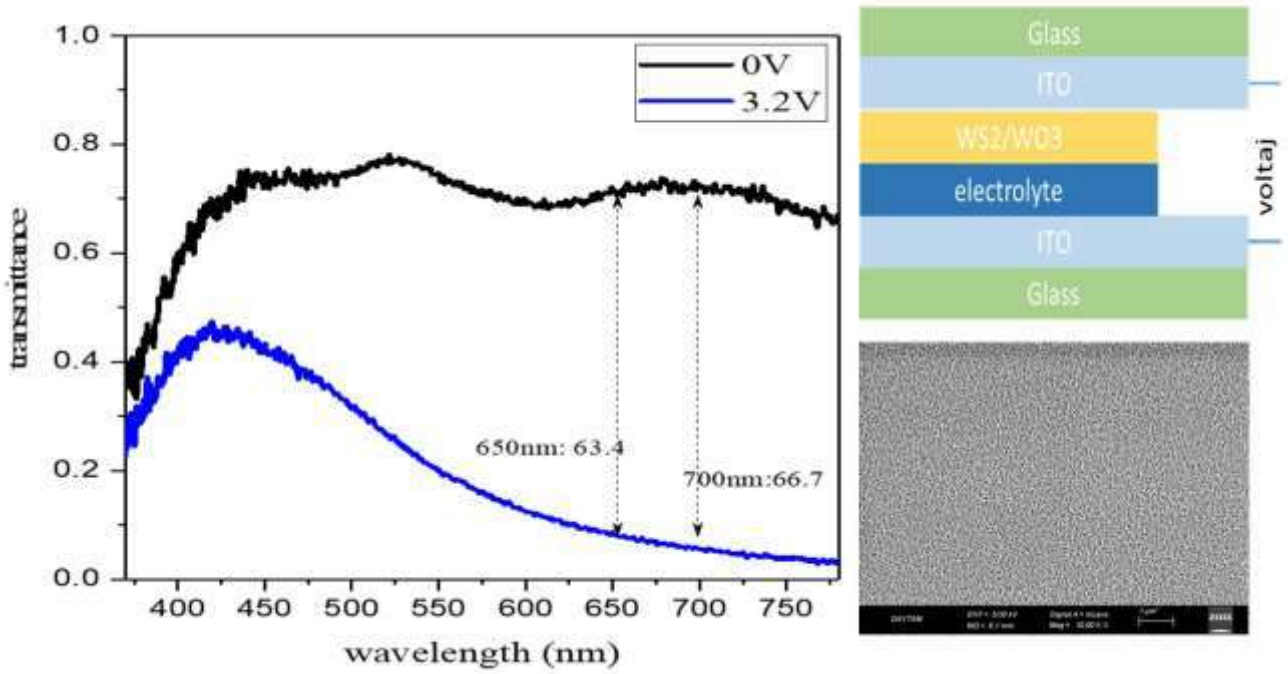

Figure 1. Electrochromic device performances of the WS_2 films converted to WO_3, device structure and nano-wall surface morphology.

Magnetically active hydrogel microenvironments for tissue stimulation

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The biomimicry of the natural microenvironment of tissues with engineered scaffolds remains one of the greatest challenges of tissue engineering. To overcome this, hydrogels are one of the most promising materials [1] due to their high water content, biocompatibility, and their ability to carry nanomaterials that grant them new and interesting properties. Specifically, incorporating polymer-based piezoelectric or magnetoelectric materials into the hydrogel allows for the creation of new hybrid scaffolds for tissue engineering applications [2]. These are capable not only of controlling the scaffold externally, by the application of magnetic fields, but also of using these same magnetic fields to promote tissue regeneration through magnetic to mechanic to electrical conversion of the initial magnetic field, allowing for piezoelectric stimuli to be directly applied to the cells [3]. In this way, this work reports on the use of electrodynamic techniques to synthetize magnetoelectric polymer composites [4], the physical characterization of these composites, the loading of the hydrogels and the evaluation of the influence of such hybrid hydrogel microenvironments on biological response. Furthermore, the possibilities of adapting these hybrid materials for different tissues will also be explored.

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References

[1] Rana D, Kumar TSS, Ramalingam M. Cell-Laden Hydrogels for Tissue Engineering. *Journal of Biomaterials and Tissue Engineering* 2014, **4**(7)**:** 507-535
[2] Ribeiro C, Sencadas V, Correia DM, Lanceros-Méndez S. Piezoelectric polymers as biomaterials for tissue engineering applications. *Colloids and Surfaces B: Biointerfaces* 2015, **136:** 46-55
[3] Martins PM, Ribeiro S, Ribeiro C, Sencadas V, Gomes AC, Gama FM, Lanceros-Méndez S. Effect of poling state and morphology of piezoelectric poly(vinylidene fluoride) membranes for skeletal muscle tissue engineering. *RSC Advances* 2013, **3**(39)**:** 17938
[4] Ribeiro C, Costa CM, Correia DM, Nunes-Pereira J, Oliveira J, Martins P, Goncalves R, Cardoso VF, Lanceros-Mendez S. Electroactive poly(vinylidene fluoride)-based structures for advanced applications. *Nat Protoc* 2018, **13**(4)**:** 681-704

Carbon nanomaterials fabricated with lipid nanotube templates

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Carbon nanomaterials have recently attracted a great deal of attention in the semiconductor industry due to their unique electrical, optical, thermal, mechanical, and chemical properties. Thus, carbon nanomaterials have gained importance in biology for applications such as biosensors and drug delivery. There is a growing interest in the use of self-assembled bioorganic templates in the fabrication of such one-dimensional carbon nanostructures.

The lipid 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (DOPE) which is the main component of bacterial cell membranes is known to self-assemble into single-wall synthetic lipid nanotubes (LNTs) on polyelectrolyte-functionalized surfaces.[1] We have demonstrated a high-throughput approach to transform these LNTs into surface attached carbon nanostructures through pyrolysis. First, biotin-tagged DOPE LNTs are formed from lipid blocks in inverted hexagonal phase adsorbed on polymer-coated surfaces upon application of shear force and cross-linked by chemical fixation.[2] Samples were dried and treated with high temperature under inert atmosphere to form connected carbon nanostructures. The created carbon nanostructures were characterized by transmission electron microscopy, atomic force microscopy and electrical measurements. The method is advantageous because the small size of LNTs enables the fabrication of surface attached mesh-like nanostructures with a higher throughput without using expensive electron beam lithography. The approach can further be combined with single LNT patterning with a micromanipulator to create distinct patterns instead of random networks.

References

[1] Sugihara et al. (2012) *ACS Nano* **6**, 6626-6632
[2] Jajcevic et al. (2016) *Small* **12**, 4830-4836

Figures

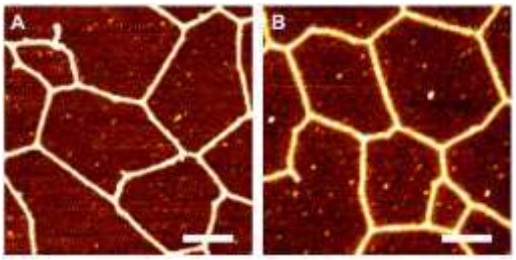

Figure 1. TEM images of surface attached LNTs before (A) and after (B) pyrolysis under inert atmosphere. Scale bars are 500 nm.

Electronic and magnetic properties of an on-surface synthesized 2D metal organic framework

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Abstract

2D MOFs constitute a new class of designer materials where the coexistence of Dirac electrons and flat bands can lead to rich physical phenomena and to the realization of quantum phases such as topological or quantum anomalous Hall insulators (1). If the metal adatom additionally bears a non-zero spin, one obtains a Magnetic Topological Insulator, where the Quantum Anomalous Hall effect can emerge.

Following the concepts of coordination chemistry (2), based on a surface-assisted self-assembly of the metal and organic components, we have carried out synthesis of Iron-hexaiminotriphenylene (HITP) MOFs on Au(111) substrate and characterized their electronic structure using scanning tunnelling spectroscopy (STS). On the other hand, ab-initio calculations of the observed structures indicate the presence of strong ferromagnetic interactions that persist under the influence of the Au substrate, indicating that the interaction with the Au substrate stabilizes even further the FM state on $Fe_3(HITP)_2$. We relate such strong magnetic interactions to the formation of a radical spin at the ligand that mediate the inter-ionic interactions.

References

[1] Z. F. Wang, Z. Liu, F. Liu, *Phys. Rev. Lett.* **110**, 196801 (2013)
[2] R. Zhang *et al.*, *Nanoscale*. **11**, 878–881 (2018)

Figures

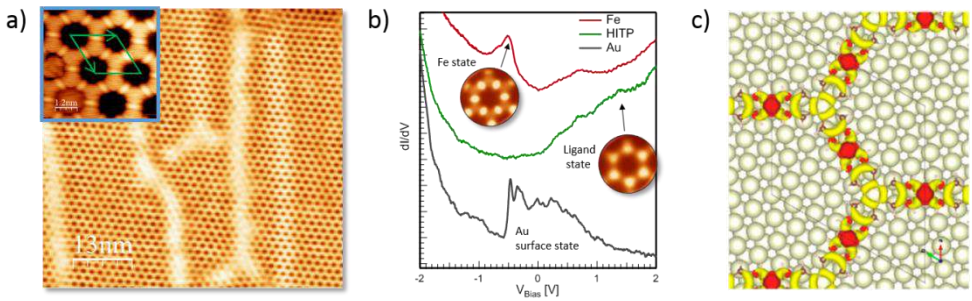

Figure 1. a) STM topographic images of $Fe_3(HITP)_2$ synthesized on Au(111). Arrows in the inset indicate the unit cell of the honeycomb structure. b) dI/dV spectra acquired at Fe and ligand sites, as well as on the clean Au surface. C) Spin density calculated for $Fe_3(HITP)_2$ on Au(111).

New hydrophobic carbon quantum dots mediated antibacterial activity in various polymer matrix

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Nowadays, there is an increasing number of bacteria resistant to a wide range of antibiotics. At the same time, the frequency of nosocomial infections is increasing. This is due to the environment in which, for example, patients are, but also due to medical devices. Bacteria have the ability to quickly settle all surfaces and survive on them incredibly long - even for years. Therefore, it is necessary to remove this problem quickly and efficiently. An effective and ecological solution is to develop new antibacterial materials based on hydrophobic carbon quantum dots (hCQDs) in polymer matrices. Such nanocomposites are working on the principle of photodynamic therapy (PDT), which is already a common part of many medical as well as cosmetic treatments. Mechanical, photophysical, chemical properties and biocompatibility (cytotoxicity, proliferation and hemolytic tests), were studied on all used materials. Gram-negative and Gram-positive bacteria were used to monitor the antibacterial effect. This material is useful in a variety of applications, such as antibacterial windows and other surfaces, catheters, fibers for antibacterial sutures on the body surface, and many others [1-2].

Acknowledgements

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References

[1] M. Kovacova, Z. M. Markovic, P. Humpolicek, M. Micusik, H. Švajdlenkova, A. Kleinova, M. Danko, P. Kubát, J. Vajdak, Z. Capakova, M. Lehocký, L. Munster, B. M. T. Markovic, Z. Spitalsky, ACS Biomater. Sci. Eng., 4, (2018), 3983−3993, DOI: 10.1021/acsbiomaterials.8b00582.
[2] Z. M. Markovic, M. Kovacova, P. Humpolicek, M. D. Budimir, J. Vajďák, P. Kubát, M. Micusik, H. Švajdlenkova, M. Danko, Z. Capakova, M. Lehocký, B. M. T. Markovic, Z. Spitalsky, Photodiagnosis Photodyn Ther., 26, (2019), 342-349, DOI: 10.1016/j.pdpdt.2019.04.019, ISSN 1572-1000.

Figures

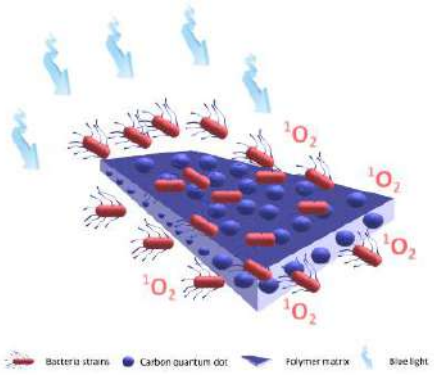

Figure 1. The mechanism of action of the polymer nanocomposite.

Hybrid BN/Au and BN/Pt nanoparticles development as promising catalysts

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INTRODUCTION

h-BN nanostructures are in focus due to a rare combination of properties. This nanostructures are considered as the key components of the next generation of advanced catalysts. The question of present interest is the development of high yield approaches for synthesis of hybrid BN/Au and BN/Pt nanoparticles for promising catalysts.

EXPERIMENTAL STUDY AND RESULTS

Different strategies of CVD process were developed for obtaining a variety of BN nanoparticles. Spherical BN nanoparticles with an average external dimensions of 80-150 nm having hollow and solid cores and smooth and petalled surfaces were synthesized using precursors on the base of FeO, MgO, SnO, H_3BO_3 and B, various temperatures and flow rates of argon and ammonia. Changing the experimental conditions affects the particle morphology, oxygen content and the product yield. The particular mechanism for each particle morphology appearance was uncovered.

BN nanoparticles composed of numerous curved nanosheets were utilized as a new catalyst support. BN/Au hybrid nanoparticles were synthesized by chemical deposition from gold chloride acid solution followed by reduction the metallic phase and also via CVD method. BN/Pt nanohybrids were obtained by chemical deposition from platinum hydrochloric acid solution followed by reduction in hydrogen flow at T=350°C. It was shown that metal nanoparticles are evenly distributed over the surface of ceramic particles and the size of metal particles does not exceed 10 nm.

Catalytic properties of nanohybrids of BN/Au and BN/Pt systems were investigated for the reaction of carbon monoxide oxidation. Synthesized hybrid nanomaterials have pronounced catalytic properties in the ratio of carbon monoxide. The best result is shown for the catalyst BN/Pt - the beginning of the conversion process was observed at a temperature of about 150°C and the temperature of the total conversion of CO was 184°C.

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Microscopic View on Relativistic Splitting and Spin-Dependent Scattering of Surface States

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Microscopic origin of the spin-orbit splitting of surface states (Rashba effect) is discussed based on *ab initio* calculations of the wave functions for realistic surfaces. The splitting is found to be primarily due to a spin-orbit induced in-plane modification of the wave function, namely, to its effect on the nonrelativistic Hamiltonian [1].

This calls for a microscopic approach to scattering of surface states from defects. Here, we present a wave-functions based method for scattering on a non-magnetic linear defect at a surface with strong spin-orbit interaction [2]. A proof-of-principle calculation for a model crystal potential demonstrates how spin-selective reflection resonances arise in scattering of Rashba-split surface states by an atomic stripe, see figure. Spin-filtering properties of such linear defects are analyzed within an envelope-function formalism for a perturbed surface based on the Rashba Hamiltonian. The continuous Rashba model provides an adequate picture and reveals the essential physics behind the scattering resonance. The spin-dependent reflection suggests a novel mechanism to manipulate spins on the nanoscale.

References

[1] E. E. Krasovskii, *Microscopic origin of the relativistic splitting of surface states*, Phys. Rev. B **90**, 115434 (2014).
[2] I. A. Nechaev and E. E. Krasovskii, *Spin filtering via resonant reflection of relativistic surface states*, Phys. Rev. B **97**, 041407(R) (2018).

Figures

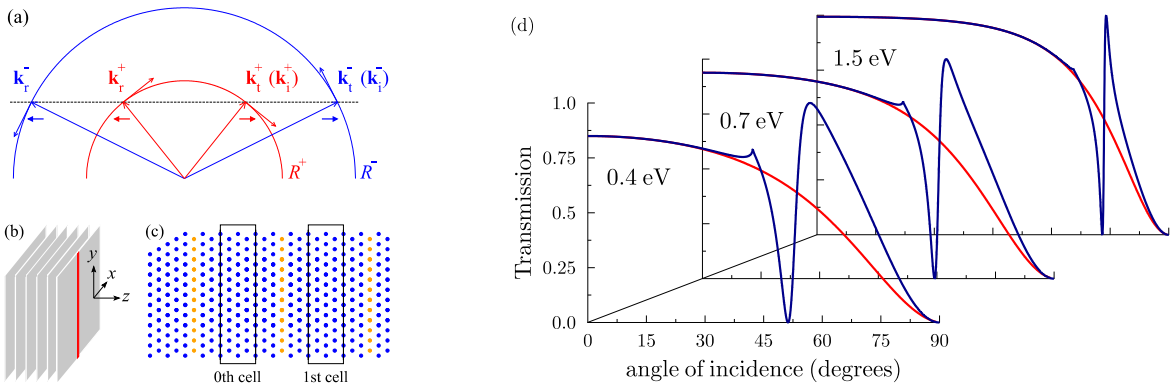

Figure 1. (a) Constant energy contours of Rashba split surface states showing incident, reflected, and transmitted waves. (b) Finite-thickness slab with a linear defect in the topmost layer. (c) Supercell geometry: topmost layer with a repeated row of impurity atoms. (d) Transmission probability as a function of the angle of incidence for $E - E_{\bar{\Gamma}} = 1.5$, 0.7, and 0.4 eV. Red and blue curves are for the incident wave in the inner and in the outer circles, respectively. The latter are seen to be fully reflected at a certain angle depending on the energy.

Synthesis of Elongated CdSe/CdS Core/Shell Nanoparticles Realized on Top of Cubic Crystal Structured Cores

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Shown here is a new and easy method to grow elongated and further more in thickness controllable CdSe/CdS core/shell nanoparticles. The particles hold a very high extinction coefficient in comparison to common core/shell structures. This made them perfect emitter materials (e.g. for display applications).

The wurtzite shell is grown on top of a cubic crystal structured core. So an elongated growth is realized without the commonly used wurtzite structured core.[1] The presented synthesis is realized using a combination of coordinating surfactantes and non coordinating solvents as well as a two step heating method.

Further studies determined the Cd to S ratio to be a main factor for the aspect ratio of the resulting particles. By now the aspect ratio can be tuned from spherical to 1:20 diameter to length, directly during the synthesis and not in post synthesis step.[2]

More over these results can be way guiding for the synthesis of elongated, cadmium free systems, because most promising materials e.g. InP or ZnSe do not exist in a the hexagonal core structure.

References: [1] L. Carbone et al., Nano Letters 7.10 (2007), S. 2942_2950

[2] M.G. Bawendi et al., ACS Nano 10, 3, (2016), S. 3295-3301

Figures:

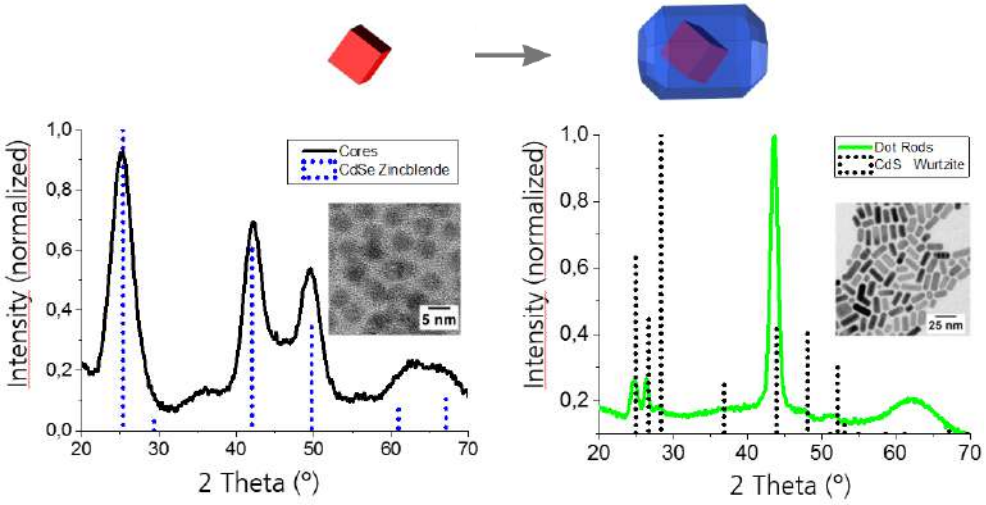

Figure 1: XRD of cubic CdSe cores (left) and resulting hexagonal CdS shell on these cores (right.)

Understanding the role of particle rigidity in nanoparticle-cellular interactions

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Engineered nanomaterials have garnered much interest in biomedical research due to their unique and tailorable properties which can facilitate spatially localised diagnostic and therapeutic effects. The interaction of medically relevant nanoparticles with biological systems is strongly influenced by a number of physico-chemical properties such as size, shape and surface chemistry [1]. While the aforementioned properties have been the subject of much study, insufficient effort has been invested in understanding the role of mechanical properties on nanomaterial bio-interactions. There is emerging evidence that particle rigidity can play a substantial role in the *in vivo* biodistribution of nanoparticles as well as their internalisation by cell subtypes [2]. In order to understand how nanomechanical behaviour impacts the biological response, we have synthesised mechanically distinct polymer microgels to explore stiffness-dependent internalisation. We assess the role of particle rigidity in two distinct arenas: internalisation from suspension, and the removal of particles from a substrate. This approach allows us to interrogate the dynamics of particle internalisation in dissimilar, but physiologically relevant models.

References

[1] C. Kinnear, T. L. Moore, L. Rodriguez-Lorenzo, B. Rothen-Rutishauser, A. Petri-Fink, *Chem. Rev* **2017**, *117*, 17, 11476-11521
[2] P. Guo, D. Liu, K. Subramanyam, B. Wang, J. Yang, J. Huang, D. Auguste, M. Moses, *Nat. Commun.* **2018**, *9*, 1, 130

Mass and stiffness nanomechanical spectrometry

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The identification of microorganisms such bacteria, viruses and fungi, is a fundamental problem in analytical chemistry and biology. Mass spectrometers (MS) identify species by their molecular mass with extremely high sensitivity (~ Da). However, reduced dynamic range (up to MDa) that is below the mass of intact microorganisms, limits conventional MS. Nanomechanical resonators have demonstrated its capacity for measuring the mass of analytes with outstanding sensitivity and high dynamic rage[1,2].
We present a mass and stiffness nanomechanical spectrometer that overcome the limitations of convencional MS. We developed a theory of the mechanical coupling between biological particles and resonant beams that predicts not only the mass but also the stiffness of the adsorbed particles by tracking the resonance frequency shifts of several vibration modes in real-time [3]. We measured gold nanoparticles, *Escherichia coli* and *Staphylococcus epidermidis* delivered by electrospray ionization to a microcantilever resonator placed in vacuum. The system is able to perfectly guide, soft-landing and focus the particles beam on the surface of the nanomechanical resonator.

References

[1] M. S. Hanay et al. Single-protein nanomechanical mass spectrometry in real time. Nature Nanotechnology, **7**, 602-608 (2012)
[2] S. D. Medina et al. Neutral mass spectrometry of virus capsids above 100 megadaltons with nanomechanical resonators, Science, 362, 918-922 (2018)
[3] O. Malvar et al. Mass and stiffness spectrometry of nanoparticles and whole intact bacteria by multimode nanomechanical resonators. Nature Communication, 7, 13452 (2016)
[4]

Figures

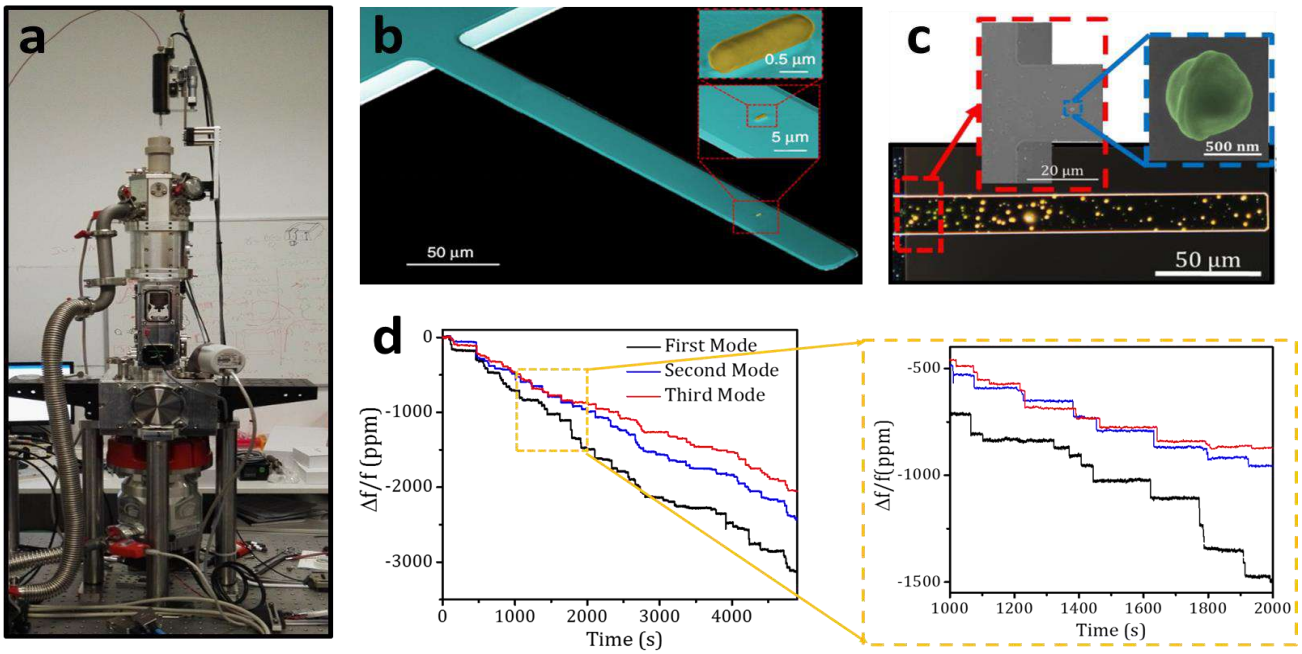

Figure 1. (a) Nanomechanical mass and stiffness spectrometer. (b) False color SEM image of an *E. coli* on a cantilever surface. (c) Dark field microscope picture of a cantilever after deposition of *S. epidermidis*. Insets show SEM images of the bacterial cells on the cantilever surface. (d) Relative frequency jumps of the first three flexural modes during an experiment.

Shaping polymer surfaces by laser interactions: formation and nanomechanical properties of LIPSS in controlled enviroments

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Laser surface patterning techniques, such as the formation of Laser Induced Periodic Surface Structures (LIPSS), have demonstrated to provide versatility and reliability, constituting a possible method to obtain large processed surface areas in polymers [1]. The formation of LIPSS can be explained as the result of the interference between the incident and the surface-scattered waves, and a positive feedback process. This leads to the formation of structures with a spatial period close to the laser wavelength, i.e., in the 100 nanometer length-scale, and aligned parallel to the polarization of the laser beam [1,2].

In this work, we report the formation of LIPSS on free-standing films of poly(ethylene terephthalate) (PET) (Figure 1). The laser structuring process was carried out in different controlled environments: vacuum, oxygen, water, and ethanol. We evaluated the formation of LIPSS by Atomic Force Microscopy (AFM) imaging. The results were always compared to those found classically for the LIPSS formation in ambient conditions (25 ºC, 50 RH%). Our AFM structural analysis showed that in vacuum, the structuring process was similar to that performed in ambient conditions. However, for the rest of the atmospheres, we found different results. For water and oxygen, we observed the formation of LIPSS, but with different geometrical characteristics. In the case of ethanol, no LIPSS were formed, although the surface of the PET films showed changes. Furthermore, following our previous work [2], we performed a nanomechanical study on the nanostructured surfaces. We used the PeakForce QNM technique, an AFM-based protocol that allows obtaining the topography, elastic modulus, and adhesion maps of the materials simultaneously. Our results are discussed taking into consideration the possible physical and chemical changes that the samples might experience during processing, as well as the changes imposed by the complex geometry of the nanometric features.

References

[1] E. Rebollar, M. Castillejo, T.A. Ezquerra, Eur. Polym. J., 2015, 73, 162.

[2] R. I. Rodríguez-Beltrán, D. E.Martínez-Tong, A. Reyes-Contreras, S. Paszkiewicz, A. Szymczyk, T. A.Ezquerra, P. Moreno, E. Rebollar. Polymer, 2019, 168, 178-184.

Figures

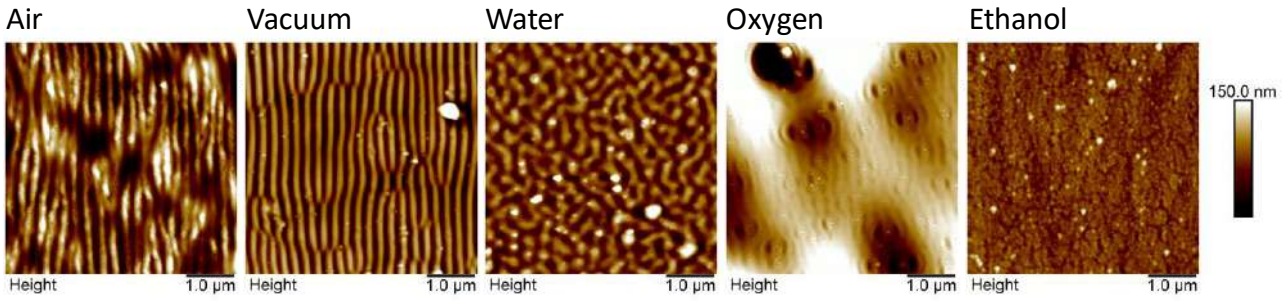

Figure 1. LIPSS on a PET free-standing film, prepared in different controlled environments.

Ab initio vibrational properties and isotope effect in H-bonded ferroelectric materials

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Motivated by the miniaturization of devices to nano levels, the interest in reducing power consumption and improving energy efficiency has continuously grown over the last years. Within this scenario, ferroelectric materials offer a wide range of useful properties, such as nonzero switchable electric polarization in the absence of an external field, piezoelectricity and pyroelectricity. This makes them promising candidates for applications such as capacitors, memories or energy harvesting devices.[1, 2]

In this work, we report the *ab initio* structural, vibrational and isotope effect properties of potassium dihydrogen phosphate (KDP or KH_2PO_4), a prototype member of the hydrogen-bonded ferroelectric compounds. A striking manifestation of its phenomenology is the huge isotope effect in its ferroelectric-paraelectric transition temperature T_c, which changes from 122K to 229K upon deuteration.

Using KDP as a case model, we have developed a novel method for selecting the exchange-correlation functional in Density Functional Theory calculations. This method incorporates quantum nuclear effects *a posteriori* in the description of the system, allowing to take them into account in the selection process. For KDP, the nonlocal van der Waals functional vdW-DF was selected as it provided the best agreement with H-bond geometries experimental data. With this choice of functional, we computed the phonon modes at the Γ point of the Brillouin zone, the phonon dispersion curves and the phononic contribution to specific heat. We were also able to calculate the electric polarization and to identify the microscopic mechanism that originates it. [3] The devised method might be useful in the study of other H-bonded materials where the isotope effect proves to be of crucial importance. [4]

References

[1] S. Pandya *et al.*, Nat. Mater. **17**, 432 (2018).
[2] T. Y. Kim *et al.*, Nano Converg. **5**, 30 (2018).
[3] R. Menchón *et al.,* Phys. Rev. B **98**, 104108 (2018).
[4] C. Shi *et al.*, Nat. Commun. **9**, 481 (2018).

Figures

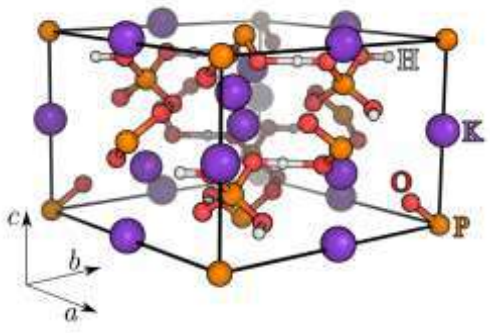

Figure 1. Schematic view of the internal structure of

Plasma Modification of Nanoporous Graphite Films

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Method of MPECVD was proposed to synthesize high porous amorphous carbon film with thin "adhesion" layer on various substrates in single cycle of the materials deposition. Annealing at high temperature in inert atmosphere leads to strong graphitization of the carbon film with significant decreasing of resistivity that allows us to consider obtained carbon films as promising material for catalysis and chemistry sensors. In this work we study plasma modification of the porous graphitizited carbon films in various gas atmospheres for enhancement of their catalytic and sensory properties.

The films were studied by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) technique and by atomic force microscopy (AFM). Wetting of the films surface was studied by the water contact angle (WCA) technique; a resistivity of the films - by four point probes method. The samples were subjected by RF (13.6 MHz) plasma treatment in hydrogen, nitrogen or argon atmosphere at room temperature in vacuum of 10^{-2} Torr.

It was shown by XRD measurements that thickness and density of the carbon film after plasma treatments are changed insignificantly and equal to about 145 nm and 1.55 g/cm^3, respectively. XPS research demonstrates incorporation of nitrogen and oxygen bonds both after hydrogen and nitrogen plasma treatment and increase concentration of sp^3 carbon bonds; after Ar plasma treatment introduction of nitrogen and oxygen was minor. Nitrogen and hydrogen plasma treatment resulted in decreasing of WCA up to 28° that attests increasing of their hydrophilicity whereas an argon plasma treatment increases of WCA up to 64° (Figure 1 (a,b)) that can be associated with specific surface morphology in last case which we observe by AFM (Figure 1 (c)). Resistivity of the hydrogen plasma treated film considerable decreases in compare with initial one while it noticeably increases after nitrogen plasma modification. Nature of the observed phenomena is analyzed and sensory properties to ammonia are estimated.

Figures

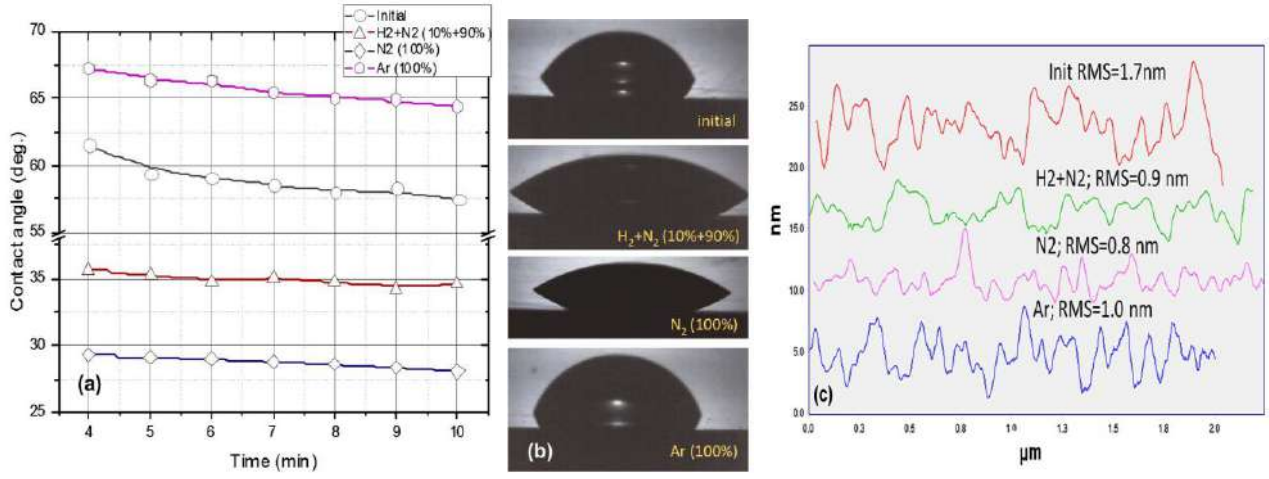

Figure 1. Water contact angle vs. time measurement after different plasma treatment (a); Photo of the drops located on grafitic surface after plasma treatment (b); Topography of graphite porous surface before and after plasma treatment measured by AFM technique.

Ab initio relativistic k·p models for non-centrosymmetric systems with competing spin-orbit and magnetic exchange interaction

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In this contribution, we present a fully *ab initio* relativistic **k·p** perturbation approach to *microscopically* generate effective Hamiltonians of a desired size [1, 2]. The approach allows one to make an effective **k·p** model capable of correctly reproducing the observable (true) spin polarization of two-dimensional (2D) states split by spin-orbit interaction (SOI) in non-centrosymmetric systems. In turn, this enables a proper treatment of the effect of magnetic exchange interaction of 2D-state electrons with a ferromagnetic substrate or supporting layer. As an example of the efficiency of our approach, in Figure 1 we show the specific SOI-induced spin polarization of the Si-terminated surface states of the rare earth (*R*) intermetallic compounds RT_2Si_2 (*T*=Ir, Rh) [2], which is characterized by a triple winding of surface-electron spins around the Fermi contours (FCs). The resulting complex spin structure underlies the shape of the FCs in the presence of the magnetic order in the rare-earth layers of RT_2Si_2. Applications of the approach to topological insulators, surface alloys, and structural elements of layered polar semiconductors are also presented in this contribution.

References

[1] I. A. Nechaev and E. E. Krasovskii, *Relativistic **k·p** Hamiltonians for centrosymmetric topological insulators from ab initio wave functions*, Phys. Rev. B **94**, 201410(R) (2016).
[2] I. A. Nechaev and E. E. Krasovskii, *Relativistic splitting of surface states at Si-terminated surfaces of the layered intermetallic compounds RT_2Si_2 (R=rare earth; T=Ir, Rh),* Phys. Rev. B **98**, 245415 (2018).

Figures

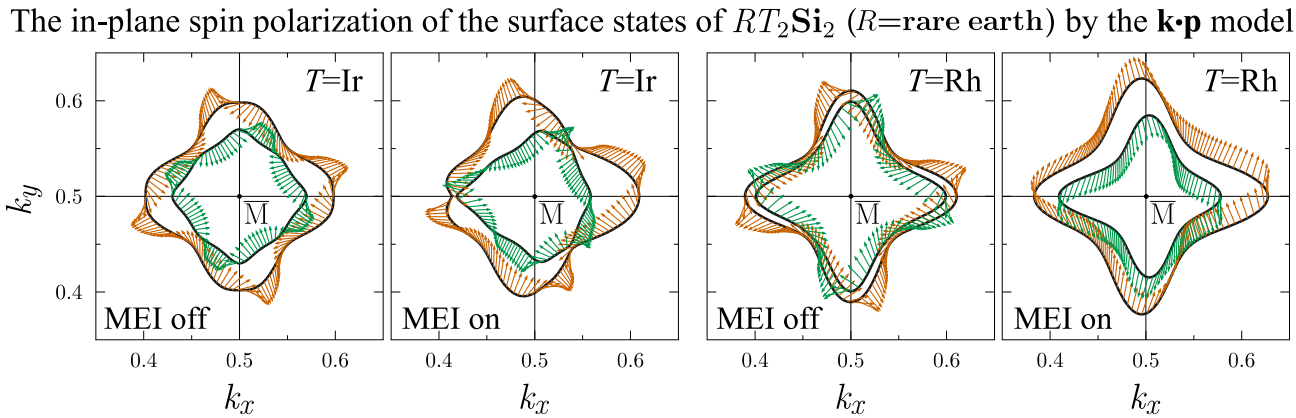

Figure 1. Spin-resolved FCs of the Si-terminated surface state of the compounds RT_2Si_2 with the in-plane orientation of the spins, $\langle \mathbf{S} \rangle = \langle S_x \rangle \hat{\mathbf{x}} + \langle S_y \rangle \hat{\mathbf{y}}$, indicated by green (orange) arrows for the inner (outer) contour. The shown FCs are obtained within a relativistic **k·p** six-band model without (MEI off) and with (MEI on) the magnetic exchange interaction of surface-state electrons with the 4*f* moments of the subsurface rare-earth atomic layer ferromagnetically ordered along the *y*-axis.

New Universal Type of Interface in the Magnetic Insulator/Topological Insulator Heterostructures

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Magnetic proximity effect at the interface between magnetic and topological insulators (MIs and TIs) is considered to have great potential in spintronics as, in principle, it allows realizing the quantum anomalous Hall and topological magneto-electric effects (QAHE and TME). Although an out-of-plane magnetization induced in a TI by the proximity effect was successfully probed in experiments, first-principles calculations reveal that a strong electrostatic potential mismatch at *abrupt* MI/TI interfaces creates harmful trivial states rendering both the QAHE and TME unfeasible in practice. Here, using density functional theory calculations, we resolve the latter problem by proposing a fundamentally new type of the interface between an MI film and a tetradymite-like TI [1, 2], which appears to be universal for binary magnetic insulators, as exemplified by MnSe/Bi_2Se_3, MnTe/Bi_2Te_3, and EuS/Bi_2Se_3. The fabrication of the proposed interface suggests a growth mechanism implying a sinking of the codeposited MI atoms into the outermost quintuple layer (QL) of the TI substrate and formation of the MnSe(Te) or EuS structure combined with few remnant atomic layers constituted the outermost QL of a TI surface: Se(Te)-Bi-Se(Te)-[MnSe(Te)]-Bi-Se(Te) or Se-Bi-Se-[EuS]-Bi-Se. Such a scenario is far more energetically favorable than that of the sharp interface formation and covalent type bonding to a TI. Strikingly, the realization of this scenario leads to a unique situation when the heterostructure's magnetic part, based on a material that intrinsically does not show van der Waals bonding (MnSe, MnTe, EuS, etc.), turns out to be van der Waals coupled to a TI substrate since the MI film is actually sandwiched between Se(Te)-Bi-Se(Te)- and -Bi-Se(Te) layers. The encapsulated magnetic film tends to adopt its bulk-like atomic structure starting already from a thickness of a few bilayers. Moreover, the total energy calculations also reveal the bulk-like magnetic ordering even for the relatively thin films inserted inside the TI QL. By adding more MI bilayers to the "grown-in" film, we have increased its thickness up to a couple of nanometers, finding each insertion to be very much energetically favorable. Altogether, this proves such systems to constitute a novel type of the MI/TI interface that provides a smooth MI-to-TI connection yielding the interface electronic structure essentially free of trivial states. These findings enable efficient engineering of the MI/TI interfaces with tailor-made properties and pave a way to realization of the QAHE and TME as well as their exotic consequences, such as image magnetic monopole or Majorana Fermions, on the basis of the MI/TI heterostructures.

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References

[1] M.M. Otrokov, T.V. Menshchikova et al. 2D Mater. **4**, 025082 (2017).
[2] S.V. Eremeev, M.M. Otrokov, E.V. Chulkov, Nano Lett. **18**, 6521 (2018).

Nanostructured graphene catalyzes the reaction between two organic molecules

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The graphene-substrate interaction can be a powerful tool to tune the electronic properties of graphene [1]. A paradigmatic example is the graphene/Ru(0001) interface. The lattice mismatch between the two systems gives rise to a strong corrugation in graphene, dramatic variations of the graphene-metal interaction, and a strong modulation of the electronic properties at the nanometer scale [2]. Furthermore the graphene/Ru(0001) interface can be used as an adsorption template for organic molecules, like TCNQ [3], due to the low reactivity of graphene. On the other hand, organic radicals (CH2-CN·) have also been employed to covalently pattern the graphene/Ru(0001) surface with high spatial selectivity [4].

In view of these results, a natural development is determining the role of supported graphene as a catalytic agent, studying the chemical reaction that may take place when multiple molecular species are adsorbed on the graphene/Ru(0001) surface. In this talk I will present our recent results on this topic [5], analyzing the adsorption of a TCNQ molecule on a graphene/Ru(0001) surface, previously functionalized with CH2-CN· radicals. By means of Density Functional Theory (DFT) calculations we determined that the graphene/Ru(0001) surface promotes the formation of TCNQ-CH2CN, in which the two molecules are bonded by means of a C-C covalent bond, a reaction that would hardly take place under non catalyzed conditions. The new TCNQ-CH2CN molecule has no magnetic moment, due to charge transfer from the surface. More interestingly, the reaction can be fully reversed by injecting electrons in the LUMO of the molecule by the STM tip. The TCNQ-CH2CN/TCNQ duo can hence be used as a reversible magnetic switch, controlled by a chemical reaction. On the other hand, our study shows that the TCNQ molecule can be used as a chemical “mop”, with which strongly bound addends can be removed from the graphene surface.

References

[1] J. Winterlin et al., *Surf. Sci.* **603**, 1841 (2009)
[2] B. Borca et al., *Phys. Rev. Lett.* **105**, 036804 (2010); D. Stradi et al., *Phys. Rev. B* **85**, 121404(R) (2012)
[3] M. Garnica et al., *Nature Phys.* **9**, 368 (2013); M. Garnica et al., *NanoLett.* **14**, 4560 (2014);
[4] J. J. Navarro et al. *Nano Lett.* **s16**, 355 (2016); J. J. Navarro et al. *Chem. Comm.* **53**, 10418 (2017).
[5] J. J. Navarro, M. Pisarra et al. *Science Advances* (2018) **4**, eaau93661

Figures

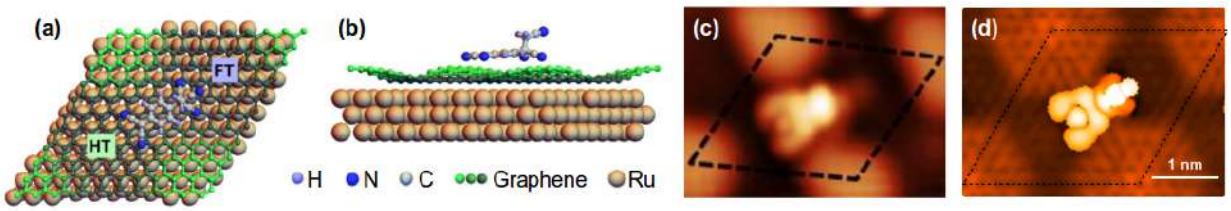

Figure 1. (a-b) Top view and side view of the unit cell including the ruthenium substrate, the corrugated graphene and the TCNQ-CH2CN molecule as obtained in the DFT calculations. (c-d) STM images of the TCNQ-CH2CN on the surface, as obtained in the STM measurements (c) and in the DFT calculations (d).

Tailoring magnetic properties of nanoparticles by gas-diffusion electrocrystallization (GDEx)

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Abstract

Gas-diffusion electrocrystallization (GDEx), a new electrochemical process that we have developed, yieds colloidal dispersions or solid nanoparticles with well controlled and narrowly distributed properties[1]. The general principles and mechanism through which GDEx operates will be introduced. Examples of nanomaterials we have achieved and their functionality and industrial relevance will be disclosed. GDEx produces finely-tuned compositions of magnetite (Fe_3O_4) nanoparticles in the range of 20 to 100 nm, providing the possibility to regulate magnetic susceptibility as MRI contrast agent and for hyperthermia treatment. Solid nanoparticles of herbertsmithite ($ZnCu_3(OH)_6Cl_2$) with liquid-like magnetic spin have also been obtained. These Cu/Zn-based nanoparticles may have applications in data storage. GDEx is revealed as a new, flexible route to synthesize a wide range of nanoparticles with versatile control of composition, morphology, and physicochemical parameters such as crystallite size, lattice parameter, particle size, which in turn tailor specific functionalities.

References

(1) Dominguez Benetton, X.; Alvarez Gallego, Y.; Porto-Carrero, C.; Gijbels, K.; Rajamani, S. An Electrochemical Process for Preparing a Compound Comprising a Metal or Metalloid and a Peroxide, Ionic or Radical Species. Patent US20180023201A1.

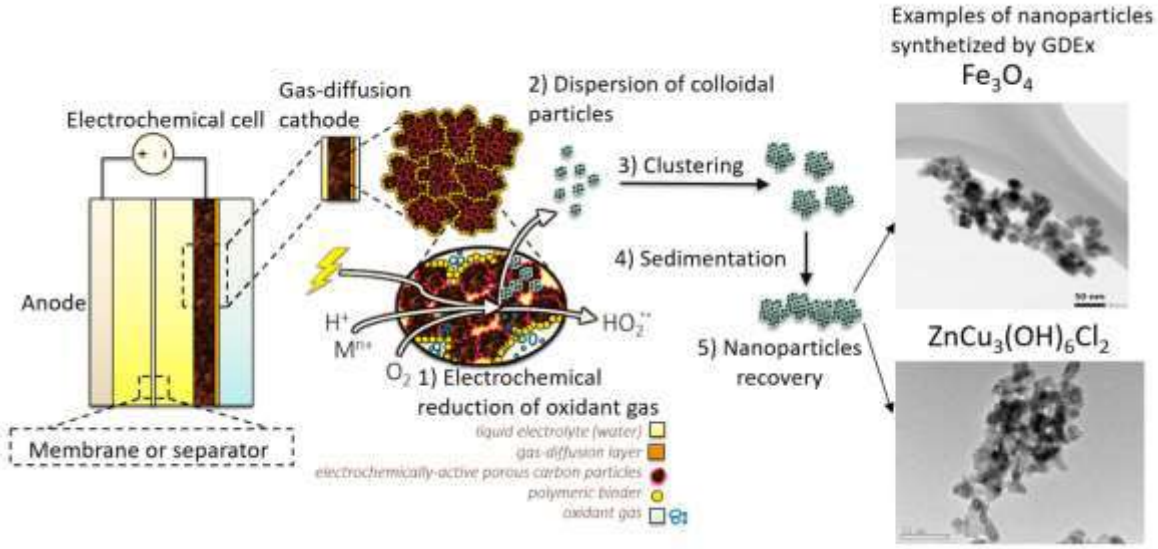

Figure 1. Gas diffusion electrocrystallization concept for the synthesis of magnetic nanoparticles.[1]

[1] **Acknowledgements** G. Pozo acknowledges the funding from the European Union's Horizon 2020 research and innovation programme MSCA-IF-2017, under grant agreement no. 796320 (MAGDEX). GP, RP, JF, and XDB thank the support from the Flemish SIM MaRes programme, under grant agreement no. 150626 (Get-A-Met project). XDB and JF thanks the funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 654100 (CHPM2030 project).

Symmetry regimes for circular photocurrents in monolayer $MoSe_2$

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The circular photogalvanic ad photon drag effects (CPGE and CPDE, respectively) are very attractive mechanisms for optically generating charge and spin transport in two-dimensional transition metal dichalcogenides (TMDCs). They allow to produce directed spin-polarized current of controllable direction and intensity by illumination with circularly polarized light, even without applying any electric bias (circular photocurrents, CPC). In this work, we study for the first time the spectral and electrical response of CPC in a monolayer TMDC. By illuminating an h-BN encapsulated monolayer $MoSe_2$ phototransistor at an oblique incidence angle with respect to the crystal surface, we generate a helicity-dependent DC photovoltage. Its dependence on the drain-source and gate voltages reveals the presence of two different CPC regimes, each becoming dominant at different applied voltages and showing different symmetry upon change of the illumination angle.

Figures

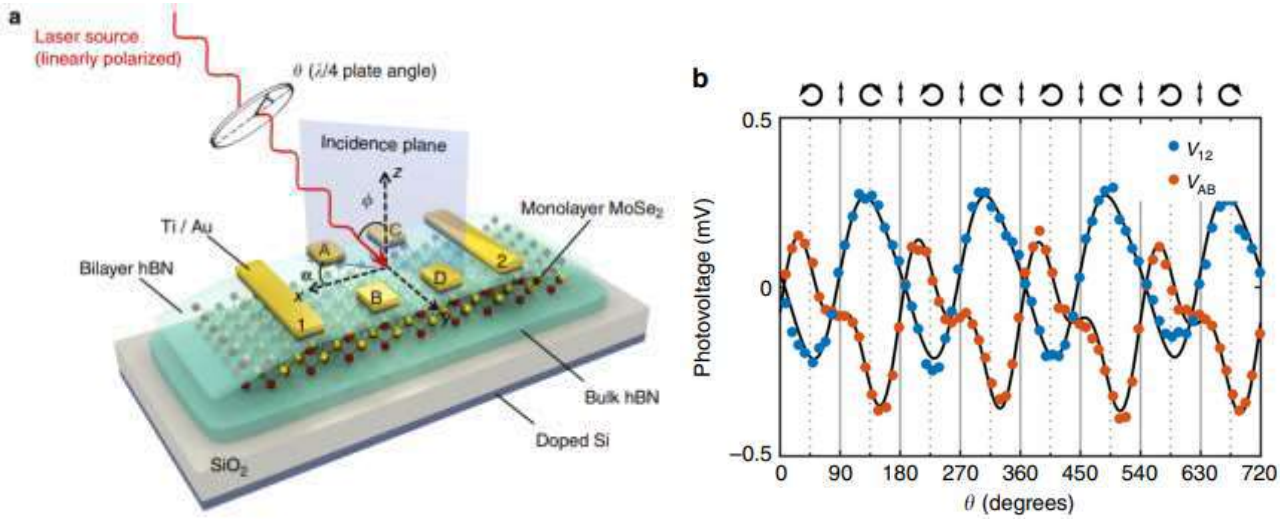

Figure. (a) Schematic experimental setup for measuring the CPGE. (b) Helicity-dependent photovoltage as a function of the quarter-waveplate angle.

SERS in the ultra-small limit: size and interparticle distance effects

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We have studied the amplification by very small Ag NPs (r=2nm) of the Raman signal from Graphene and Rhodamine 6G (R6G). The Ag NPs, deposited on glass with a gas aggregation technique, present a very narrow size distribution (2 ± 2 nm) and surface free of organics. We have evaluated the suitability of ultra-small Ag Np as SERS[1] substrate. Although the electric field amplification factor for isolated ultra-small NPs is hampered by size effects[1,2], the increase in the density of available hotspots[2] may benefit the overall amplification for organic molecules.

We present experimental results on the dependence as a function of the NPs density of the plasmon and of the Raman amplification factors for an underlying SL graphene and for spin coated R6G. Numerical simulations (Lumerical FDTD Solutions) of close-packed NPs are used to reproduce the experimental results and obtain general trends. The observed energy and shape modifications of the plasmon are not related to the NPs size distribution, very narrow in this case, but to the presence of interacting NPs with varying distributions of inter-particle distances as their density is increased. The obtained amplification factors for these 2 nm NPs (when normalized to the silver mass present in the platforms) is higher than those corresponding to larger (r= 10-15 nm) Ag Nps. The amplification for R6G increases exponentially with NPs density due to the enhanced electric fields as the inter-particle distance is reduced, being larger at the equatorial planes of the NPs (Figure), where some R6G may be present, this effect however doesn't affect the Raman signal of the underlying graphene.

References

[1] Schatz G.C., Young M.A., Van Duyne R.P. (2006) Electromagnetic Mechanism of SERS. In Surface-Enhanced Raman Scattering. Topics in Applied Physics, vol 103. Springer

[2] Ref Ultrahigh-Density Array of Silver Nanoclusters for SERS Substrate with High Sensitivity and Excellent Reproducibility. Won Joon Cho, Youngsuk Kim, and Jin Kon Kim *ACS Nano* **2012** *6* (1), 249-255

Figures

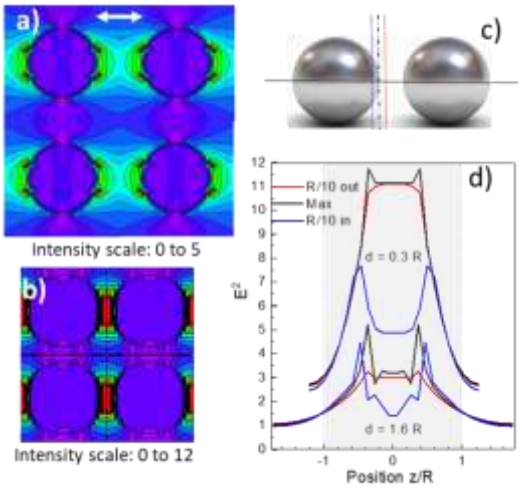

Figure 1. Electric field amplification of a periodic array of Ag NPs for to interparticles distances.

On-Surface Site-Selective Chemical Conversions -- Corroles on Ag(111)

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The electronic structure of flexible macromolecules like corroles promotes the stabilization of metal ions in exceptionally high oxidation states. This makes them distinctive candidates for various biomedicine, catalysis, as well as solar cell applications.
Combining *first-principles* calculations, temperature-programmed desorption (TPD) measurements, scanning tunneling microscopy (STM), X-ray spectroscopy (XPS), near-edge X-ray absorption fine structure (NEXAFS) spectroscopy measurements and simulations, we characterize the chemical state and the conformation of the free-base corrole 5,10,15-tris(pentauorophenyl)corrole (3H-TpFPC) adsorbed on Ag(111) surface and unravel annealing induced chemical reactions. With our novel method to simulate the XPS and the angle dependent NEXAFS signatures of the C1s and N1s edges, we can interpret the spectral features and predict the temperature induced new molecular chemical states. [1]
We reveal a formation of on-surface stable corrole radicals by a site-specific cleavage of a pyrrole N-H bond triggered by annealing to 330 K. The molecular species adsorb with their macrocycle tilted approximately 20° with respect to the surface plane contrasting the typical saddle-shape conformation of related porphyrin species. The tilted adsorption geometries enable the molecules to aggregate in non-trivial interwoven monolayer structures. [1,2] After annealing to 430 K, a thermally induced regioselective cyclization (ring closure) reaction, between the phenyl ring and the pyrrolic moiety, mediated by the radical cascade has been reported. The ring-closed radicals form a highly symmetric hexagonal monolayer structure. [3] Our calculations resolve the packing motif and predict the molecular conformations within the structure, which might offer exciting areas of application.

References

[1] H. Aldahhak, et al., J. Phys. Chem. C, 121, 2192, 2017.
[2] S. Tebi et al., ACS nano 11, 3383, 2017.
[3] H. Aldahhak, et al., Chem. Euro. J. 24, 6787, 2018.

Figures

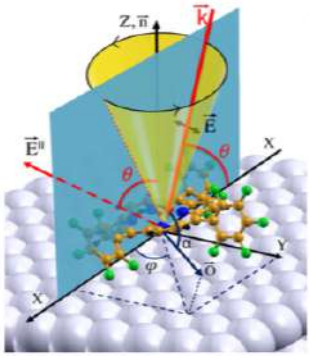

Figure 1. NEXAFS in experiment and simulations for structure identification

Mesoscopic valley filter in graphene Corbino disk containing p-n junction

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The Corbino geometry allows one to investigate the propagation of electric current along a p-n interface in ballistic graphene in the absence of edge states appearing for the familiar Hall-bar geometry. Using the transfer matrix in the angular-momentum space we find that for sufficiently strong magnetic fields the current propagates only in one direction, determined by the magnetic field direction and the interface orientation, and the two valleys, K and K', are equally occupied. Spatially-anisotropic effective mass may suppress one of the valley currents, selected together with the direction of propagation, transforming the system into a mesoscopic version of the valley filter. The filtering mechanism can be fully understood within the effective Dirac theory, without referring to atomic-scale effects which are significant in proposals operating on localized edge states.

Figures

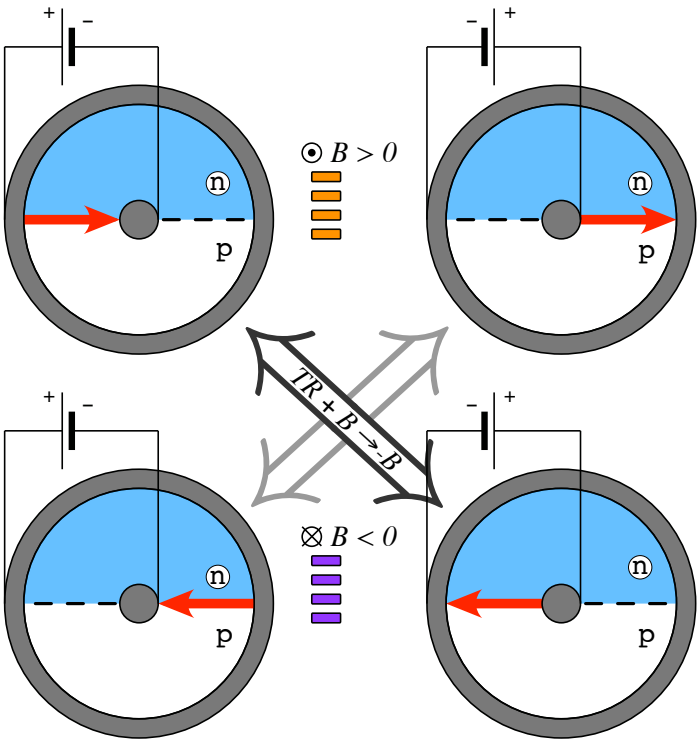

Figure 1. Quantum Hall states propagating along a p-n junction in the strong-field limit, for B > 0 (top) and B < 0 (bottom). Diagonal double arrows indicate the system symmetry upon a simultaneous time reversal and magnetic field inversion.

p-type-doped WSe_2 nanoelectronic devices fabricated by oxidation scanning probe lithography

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Oxidation Scanning Probe Lithography (o-SPL) is a direct, robust nanolithographic technique with sub-10 nm resolution and in-situ, non-destructive inspection after nanopatterning. The fabrication of working nano-devices on a wide variety of materials has been demonstrated [1]. In this work [2], we report the fabrication of 10 oxide nanowires with 36 nm half-pitch and the electrical characterization of a few-layer, p-type doped WSe_2 field-effect transistor, which channel consists in an array of 5 parallel nanoribbons with a half-pitch of 350 nm. The p-doping effect and the ability to control the width and the depth of the oxide nanoribbons come from an oxygen plasma treatment, prior to the o-SPL step, which forms a self-limited and uniform oxide layer on top of the WSe_2 flake. These results show the potential to optimize o-SPL to fabricate in a local and non-invasive way high-resolution 2D materials-based devices.

References

[1] Y. K. Ryu and R. Garcia, Advanced oxidation scanning probe lithography, **Nanotechnology** (2017), **28**, 142003.
[2] A. I. Dago, Y. K. Ryu, F. J. Palomares and R. Garcia, Direct patterning of p-type-doped few-layer WSe_2 nanoelectronic devices by oxidation scanning probe lithography, **ACS Applied Materials and Interfaces** (2018), **10**, 40054.

Figures

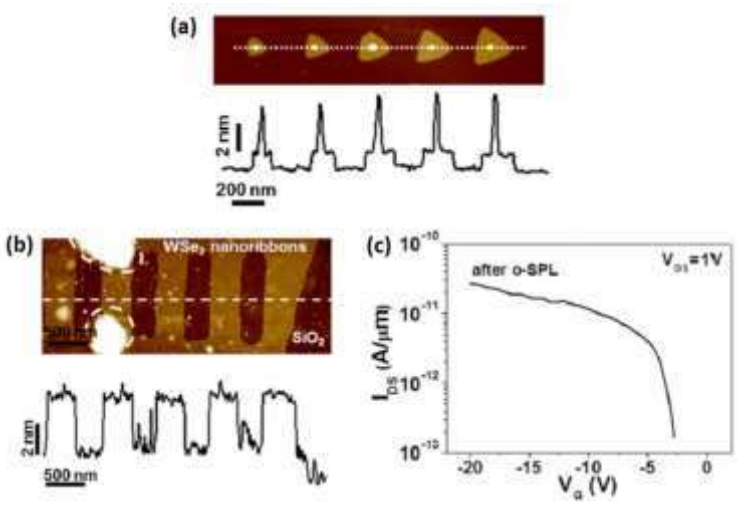

Figure 1. (a) o-SPL oxides fabricated on a pristine WSe_2 flake at arelative humidity of 42%, an applied voltage of 16.2 V and variable oxidation times in the range of 0.6 – 1.8 ms. (b) AFM topographic image of 350 nm half-pitch nanoribbons after o-SPL and water etching. (c) Transfer curve of the device shown in (b).

Oxide Nanosheets Structured Upconverting Nanofilms

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The lanthanide-doped upconversion nanomaterials have a nonlinear optical process involving sequential absorption of two or more photons leading to the emission of higher energy photons. These nanomaterials, because of their intriguing luminescent properties cover diverse applications such as solar cells [1], tissue engineering [2], safety inks [3] and display devices [4]. Single crystalline inorganic nanosheets, a class of 2D materials, are synthesized by chemical exfoliation of layered oxide materials. They are obtained from one-to-several nanometers thick depending on the composition of host layers of bulk materials. In this study, $K_2Ln_2Ti_3O_{10}$ (Ln: lanthanide), the Ruddlesden-Popper type perovskite, were doped with la Yb^{3+}/Er^{3+}, Yb^{3+}/Tm^{3+}, and Tm^{3+}/Er^{3+} ion pairs and then exfoliated to produce upconversion crytallines. These nanosheets were deposited by the layer-by-layer method to fabricate upconverting nanofilms having ~50 nm thickness. These nanofilms show emission in different parts of the visible region by upconversion depending on the amount of doping with lanthanides and the annealing temperature of the layered materials. The characterization of the layered materials, nanosheets and nanofilms were performed using Atomic Force Microscopy, X-ray Diffraction Spectroscopy, Scanning Electron Microscopy-EDX and UV/VIS/NIR Spectroscopy techniques.

References

[1] Zou, W., Visser, C., Maduro, J. A., Pshenichnikov, M. S., Hummelen, J. C. (2012). Broadband dye-sensitized upconversion of near-infrared light. Nature Photonics, 6(8), 560.
[2] Chen, G., Shen, J., Ohulchanskyy, T. Y., Patel, N. J., Kutikov, A., Li, Z., Song, J., Pandey, R. K., Ågren, H., Prasad, R. K., Han, G. (2012). (α-$NaYbF_4$: Tm^{3+})/CaF_2 core/shell nanoparticles with efficient near-infrared to near-infrared upconversion for high-contrast deep tissue bioimaging. ACS Nano, 6(9), 8280-8287.
[3] Zhao, J., Jin, D., Schartner, E. P., Lu, Y., Liu, Y., Zvyagin, A. V., Zhang, L., Dawes, J.M., Xi, P., Piper, J. A., Goldys, E. M., Monro, T.M. (2013). Single-nanocrystal sensitivity achieved by enhanced upconversion luminescence. Nature Nanotechnology, 8(10), 729.
[4] He, M., Li, Z., Ge, Y., Liu, Z. (2016). Portable upconversion nanoparticles-based paper device for field testing of drug abuse. Analytical Chemistry, 88(3), 1530-1534.

Acknowledgments

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Structure and electronic properties of h-BN on curved crystals

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The structural and electronic properties of hexagonal boron nitride (h-BN) grown on stepped Ni and Rh surfaces are systematically investigated using cylindrical Ni and Rh crystals as a tunable substrate. Our experiments reveal homogeneous h-BN monolayer coating of the entire curved surface, which in undergoes an overall faceting on Ni with large facets but h-BN nanoribbon growth on Rh.

The faceted system on Ni is defined by step-free h-BN/Ni(1 1 1) terraces alternating with strongly tilted h-BN/Ni(1 1 5) or h-BN/Ni(1 1 0) nanostripes, depending on whether we have A-type or B-type vicinal surfaces, respectively. Such deep substrate self-organization is explained by both the rigidity of the h-BN lattice and the lack of registry with Ni crystal planes in the vicinity of the (1 1 1) surface. The analysis of the electronic properties by photoemission and absorption spectroscopies reveal a weaker h-BN/Ni interaction in (1 1 0)- and (1 1 5)-oriented facets, as well as an upward shift of the valence band with respect to the band position at the h-BN/Ni(1 1 1) terrace [1].

h-BN growth on stepped Rh leads to a transformation of the two-dimensional “nanomesh” structure [2] characterized by hole and wire areas to a formation of h-BN nanoribbons where the width of the nanoribbon is tunable by the substrate vicinal angle. We find faceting of the substrate into (1 1 2) and (1 1 3) surfaces, where interaction with the Rh substrate increases (contrary to Ni). Furthermore h-BN band gap openings due to the limited nanoribbon width are observed.

References

[1] L Fernandez et al. 2D Mater. 6 (2019) 025013.
[2] M. Corso et al. Science 303 (2004) 217.

Figures

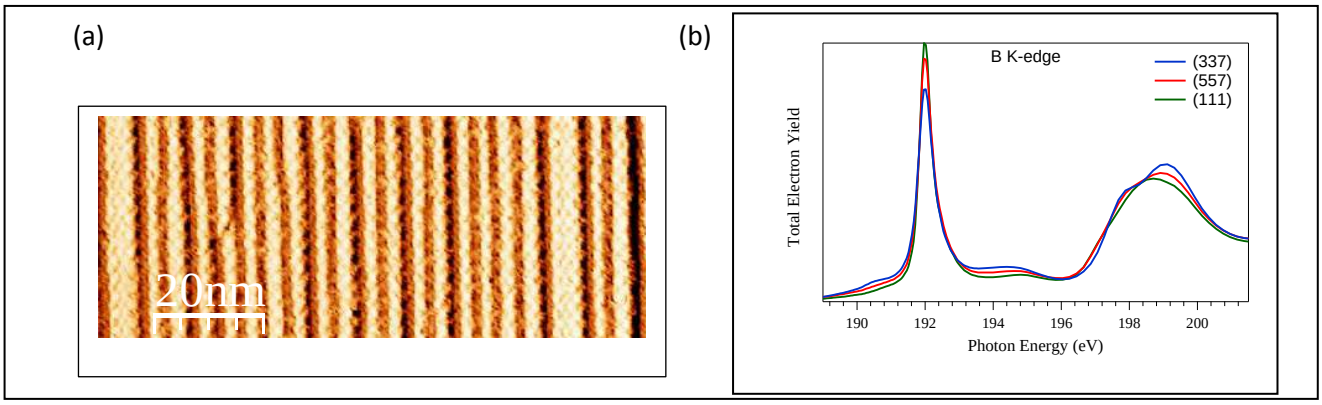

Figure 1: **(a)** STM image of hBN nanoribbons at Rh(557), **(b)** X-ray absorption spectra at the boron K-edge of a h-BN film away from the Rh(111) position of the curved crystal revealing the stronger substrate interaction.

Lock-in thermography to investigate nanomaterial-cell association trends

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The characterization of nanomaterials (NMs) in complex environments are prominent research interests in nanotechnology. Applied methods must be capable of analyzing nanomaterials with various sizes, shapes and chemical compositions. When those NMs are e.g. exposed to a cellular environment they will likely be associated and uptaken by cells. Common techniques to investigate NM-cell interactions include e.g. inductively coupled plasma mass spectrometry (ICP-MS), electron microscopy (EM) or laser scanning microscopy (LSM). However, all these methods have their limitations, e.g. time-consuming sample preparation and measurements or sample destruction [1]. Therefore, new complementary approaches are being developed. Lock-in thermography (LIT) is a sensitive infrared imaging technique, which is commonly used to test composites and electronic components [2]. The method allows analysis of stimuli-responsive samples by applying a trigger to excite NPs, resulting in the generation of heat [3]. Sample preparation is straight-forward and solid as well as liquid samples can be investigated in a non-destructive and non-intrusive way. We used LIT to stimulate plasmonic gold nanoparticles (AuNPs) and multiwalled carbon nanotubes (MWCNTs), which we exposed to different cell types for 24 hours. Homogeneous light of a specific wavelength was applied to excite these nanomaterials. The result is a 2D heat map, which allows quantifying the produced heat with respect to the applied light intensity. Hence, we gain insights in the degree of NM-cell association over the course of 24 hours by measuring at different time points.

References

[1] Mourdikoudis et al., *Nanoscale* 2018, 10, 12871.
[2] Huth et al., *Solid State Phenom.* 2002, 82–84, 741.
[3] Monnier et al., *Nanoscale* 2016, 8, 13321.

Figures

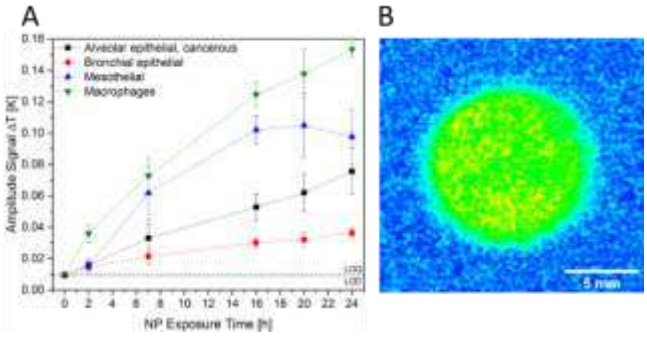

Figure 1. NM-cell association trends for different cell types over 24 hours (A) and 2D heat map obtained by lock-in thermography measurements (B). Feedback on the NM-cell association rate can by drawn by analyzing the characteristic heating behavior of NMs at different exposure time points. High temperatures are depicted in red (B).

High lateral resolution fibered sensor for dosimetry at high energies

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Abstract

X-rays are nowadays essential in the characterization and metrology of materials, objects and living species as well as in cancer therapy. The industrial development of X-ray detectors and cameras is however still hindered by the difficulty to ensure efficient “X-photon”-to-electron conversion in electronic devices needed to reach high signal/noise ratio. Indirect detection technique, which combines scintillators to silicon-based optical detectors, has demonstrated performances in terms of image contrast and signal dynamics, and are now widely developed by many companies. However, problem remains that the resulting sensors and cameras suffer from modest spatial resolution (about 10 µm) and cross-talk between neighboring pixels. Best resolution up to 1.6 microns is achieved with cameras which incorporate expensive and high steric hindrance bulky lens. On the other hand, X-ray detectors and cameras are often too bulky to allow easy manipulation, rapid implementation into systems, and endoscopic for in-vivo applications.
The purpose of our study is to show the feasibility, to design and to test the performances of novel extremely compact and highly sensitive X-ray micro and nano-detectors grafted at the end of single optical fibers [1]. The main idea is to take advantage of a new Nano-Optical Antenna (NOA) for efficiently collecting and transferring X-ray Excited Photoluminescence (XEP) from nanoscintillators towards optical fiber aperture (figure 1), in order to achieve high performance X-ray detectors and cameras available in compact and flexible architectures free from bulky optics and compatible with endoscopy (see fig.1).

References

[1] Z. Xie et al., Optics Letters, Vol. 42(7), 1361-1364 (2017)

Figures

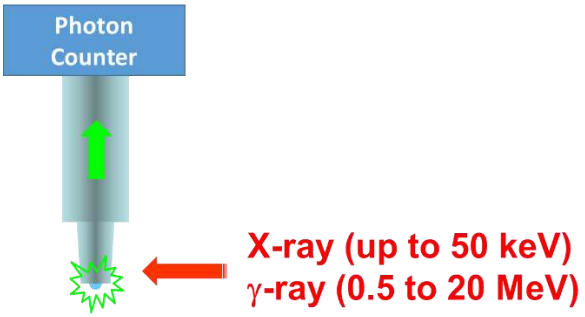

Figure 1. Test bed for simulation results validation

Magnetoresponsive nanosystems with controlled morphology and surface functionalization

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The development of magnetic nanostructures for various applications requires control of the important characteristics of these materials: morphology and size, colloidal stability, surface properties and to ensure high magnetic moment. We report a comparative study of magnetic nanosystems with tunable size, morphology, magnetic and surface properties designed for applications in magnetic bioseparation, nanomedicine, security. Design of magnetoresponsive nanocomposites was achieved using different synthesis procedures that allow either controlled clustering of magnetic nanoparticles embedded into polymers or single-core magnetite nanoparticles coated with specific functionalized shells [1-3]. The coating of individual magnetite nanoparticles with various polymeric shells (polyesters, polydopamine) allows linking additional functions for attachment of biological entities like biotine, galactose. Multi-core magnetic particle systems coated with different polymers: (poly(N-isopropylacrylamide), polyacrylic acid, poly(3-acrylamidopropyl)-trimethylammonium chloride), poly(vinylpyrrolidone), polyethylene glycol or Pluronic 68 have been obtained by miniemulsion or solvothermal methods. TEM investigations show the close packing of magnetite nanoparticles into well-defined spherical microgel particles with sizes in the range 50-300 nm, while for core-shell nanostructures the magnetic core (mean diameter 10 – 30 nm) is covered with a polymeric shell. X-ray Photoelectron Spectroscopy investigation of surface chemical composition of the magnetic microgels and core-shell nanostructures confirms the nanocomposites formation and the attachment of specific functionalities. The magnetic nanocomposites show superparamagnetic behavior at room temperature and relatively high saturation magnetization values (50-90 emu/g). Our results show that optimizing the composition, structure and functional coatings of magnetic nanoparticle systems is a great promise for the design and reproducible manufacturing of single- and multi-core magnetoresponsive nanocomposites for specific applications.

References

[1] R. Turcu, V. Socoliuc, I. Craciunescu, A. Petran, A. Paulus, M. Franzreb, E. Vasile, L. Vekas, Soft Matter 11 (5), 1008-1018 (2015)
[2] A. Bunge, A. S. Porav, G. Borodi, T. Radu, A. Pîrnău, C. Berghian-Grosan, R. Turcu, Journal of Materials Science 54(4), 2853-2875 (2019)
[3] A. Nan, T. Radu, R. Turcu, RSC Advances 6, 43330 (2016)

Figures

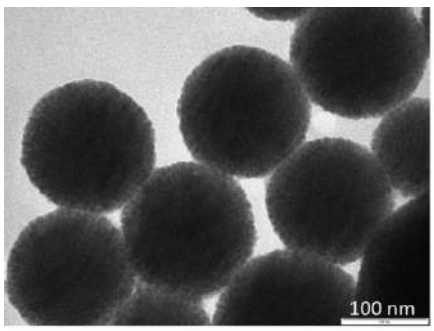

Figure 1. TEM image of magnetic clusters obtained by oil-in-water miniemulsion technique using highly stable ferrofluid.

Applications of hybrid graphene pastes for functional printing

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Functional printing enables new business lines applied to diverse sectors such as industrial sector (circuits, antennas, sensors, batteries, etc.), the agri-food sector (bio-sensors, smart packaging and labels, etc.) or the health sector (biochemical diagnosis devices, biological testing, etc.). In this work we present several applications currently under development based on functional graphene pastes combined with silver nanowires.

The excellent thermal and electrical properties of graphene spread heat rapidly, this together with the piezoresistive behaviour of graphene opens the field to novel devices, like efficient heating elements, pressure sensors or structural health monitoring. Moreover, graphene's large surface area, high electrical conductivity, unique optical properties and high thermal conductivity make it especially ideal for sensors. Ultra-sensitive graphene-based sensors can also be smaller, lighter and less expensive than traditional sensors.

The following functionalities will be presented. (a) Heating elements. Temperatures in the range of 80ºC-160 ºC are achieved with voltages between 20-30 V. Good behaviour after long cycles, reaching the same temperatures in each cycle (b) Structural health monitoring. Gauge factors up to 30 have been reached in steel samples coated with different graphene-based materials when subject to mechanical strain. (c) Pressure sensing. Preliminary results of bending tests on printed textiles show good correlation between curvature ratios and resistivity; behaviours in long time cycles. (d) Temperature sensing. Screen printed sensors based on resistive graphene-pastes integrated in a Wheatstone bridge show high sensitivity and quick answer.

The potential industrial applications will be also presented.

Figures

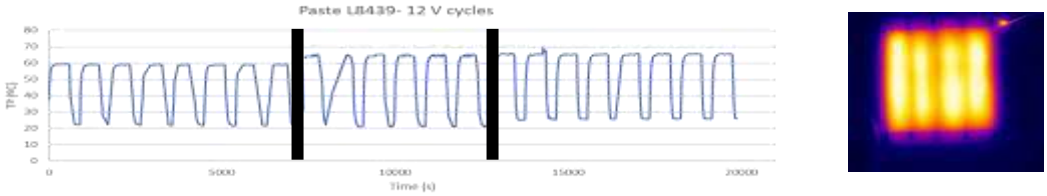

Figure 1. Electrothermal behaviour of printed graphene paste after several cycles

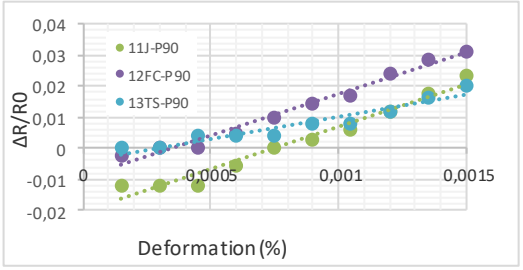

Figure 2. Piezoresistive behaviour of several graphene pastes

Figure 3. Temperature sensor

Ferrofluids and ferrofluid based magnetorheological fluids: tuning the flow behavior by micron-size Fe particles and magnetite nanoclusters

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The flow behavior of practically structure-less ferrofluids was tuned over a large range by adding well-defined amounts of magnetite nanoparticle clusters. Magnetite nanoparticle clusters with hydrophobic coating were dispersed in high colloidal stability transformer oil based ferrofluid samples having 120 and 500 G saturation magnetization, initially free of clusters. The resulting ferrofluid composition consists both of single (approx. 7 nm mean size) and clustered (280 nm average size) magnetite nanoparticles, each of them in a prescribed amount. This new approach allows a precise evaluation of the role of clusters on the ferrofluid flow behavior. The magnetite nanoparticle clusters obtained by a solvothermal method have a saturation magnetization of 75 emu/g and a remnant magnetization of 0.2 emu/g due to the large size (~25nm) of the magnetite nanoparticles in their composition. Long bundles of thin elongated needle like aggregates of magnetic nanocluster particles are formed in a magnetic field and produce a significant magnetorheological response of the bidisperse magnetic suspensions observed already for moderate applied magnetic field values (fig.1). The dynamic yield stress and magnetoviscous (MV) effect are analyzed and compared with previous results concerning suspensions of micrometer size iron particles in a ferrofluid carrier [1]. The viscoelastic properties and the interactions between the components of ferrofluid based magnetite nanoparticle cluster suspensions were evaluated by creep tests in zero and nonzero applied magnetic field. The bidisperse magnetic nanocomposite suspensions provide a promising new formulation of MR fluids with improved kinetic stability to be used in seismic dampers and flow control devices for hydraulic machinery.

References

[1] Susan-Resiga D., Vekas L., *Ferrofluid based composite fluids: Magnetorheological properties correlated by Mason and Casson numbers*, Journal of Rheology, 61, 401-408 (2017)

Figures

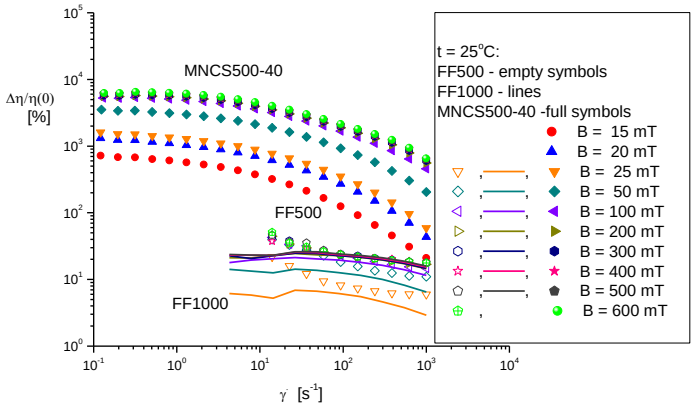

Figure 1. The MV effect of: a) MNCS120-5 and FF120, b) MNCS120-10 and FF120, c) MNCS500-10, FF500 and FF600, and d) MNCS500-40, FF500 and FF 1000 at several values of the applied field magnetic field

Broad band infrared modulation with spintronic-plasmonic metasurfaces

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Giant Magneto Resistance (GMR) materials have been incorporated into the list of candidates for active-control, demonstrating modulation of mid-IR response in spintronic-plasmonic platforms using very low magnetic fields [1, 2]. This is due to the change in the optical response induced by the magnetic field as a result of the change in electrical resistivity (Magneto Refractive Effect or MRE), which enables fast and contactless modulation of the optical properties of the spintronic material in the IR and longer wavelengths. We experimentally demonstrate and theoretically confirm that metasurfaces consisting of arrays of randomly distributed slits fabricated on $Ni_{81}Fe_{19}$/Au multilayers exhibiting 4.2% GMR, show spintronic modulation of their optical properties in the 2-17 μm range of the spectrum, using very low magnetic fields. We find a continuous increase of the modulation of the optical reflectivity with both the slit concentration and the slit length and a red-shift of the plasmon peak position at which the modulation takes on for longer slits. These results open a route to design active metasurfaces covering different spectral regions (mid-far IR, THz, GHz...), by simply adapting the size and shape of the building blocks and their spatial distribution.

References

[1] G. Armelles et al., Opt. Express 25, 18784 (2017).
[2] G. Armelles et al., ACS Photonics 5, 3956 (2018).

Figures

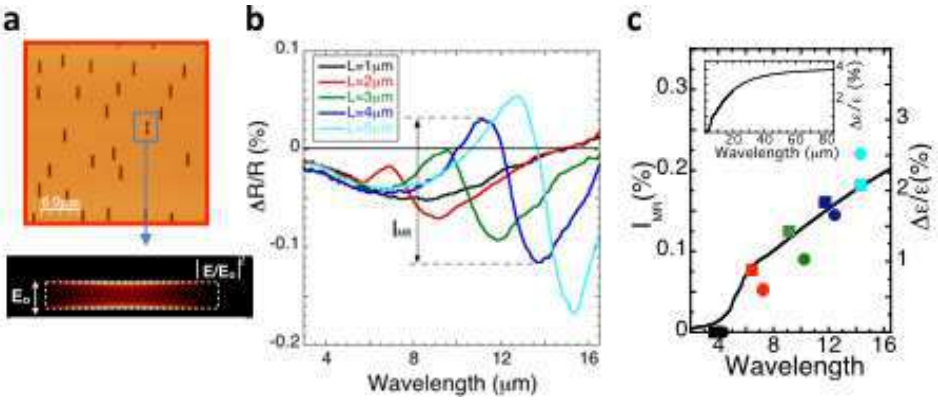

Figure 1. a) AFM image of slit metasurface (2.1% and L=2μm) and field enhancement, b) magnetic modulation for slits of different lengths and c) experimental (dots) and theoretical (squares) amplitude of magnetic modulation (I_{MR}). Black curve: magneto-induced variation of dielectric constant due to MR effect.

Synthesis of Ultrathin Silver Nanorods and Enhancing Their Stability in Biofluids

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Abstract
Silver nanorods are commonly believed to exhibit better optical performance comparing to their gold counterparts. However, in the past two decades, they have received much less attention than gold nanorods in the field of plasmonics and related interdisciplinary fields. A main drawback for practical applications of silver nanorods is the poor chemical and structural stability. In particular, the toxicity of silver ions, as a result of silver degradation, largely hinders their applications in biological analytics based on cell cultures. Another drawback is a lack of facile synthetic methods, especially for thin silver nanorods with diameters below 20 nm. We herein report a robust synthetic method for the preparation of ultrathin silver nanorods with controllable diameters of 10–20 nm and widely tunable lengths ranging from a few tens of nanometers to several micrometers. Penta-twinned gold nanoparticles are used as seeds to direct the growth of silver nanorods.[1,2] Depending on the sizes of the gold seeds, symmetric or asymmetric nanorods can be obtained due to a size dependent effect of heterogeneous/homogeneous silver overgrowth. These ultrathin silver nanorods possess a number of attractive features, including highly tunable plasmon wavelengths, intensive local field enhancement, outstanding dimensional uniformity, narrow plasmon bands, excellent photo-thermal conversion ability, and promising sensing performance. Furthermore, they are demonstrated to be stable and noncytotoxic after coating with a thin layer of polymer, where Raman molecules and dye molecules can be also facilely loaded inside. Intracellular surface-enhanced Raman scattering (SERS) imaging and surface-enhance fluorescence imaging are performed as examples for demonstrating the potential applications and outstanding performance of the ultrathin silver nanorods.

References

[1] A. Sánchez-Iglesias, N. Winckelmans, T. Altantzis, S. Bals, M. Grzelczak, L. M. Liz-Marzán. High-Yield Seeded Growth of Monodisperse Pentatwinned Gold Nanoparticles through Thermally Induced Seed Twinning. *J. Am. Chem. Soc.* **2017**, *139*, 107−110.

[2] X. L. Zhuo, X. Z. Zhu, Q. Li, Z. Yang, J. F. Wang. Gold Nanobipyramid-Directed Growth of Length-Variable Silver Nanorods with Multipolar Plasmon Resonances. *ACS Nano* **2015**, *9*, 7523−7535.

[3] D. Jimenez de Aberasturi, A. B. Serrano-Montes, J. Langer, M. Henriksen-Lacey, W. J. Parak, L. M. Liz-Marzán, L. M. Surface Enhanced Raman Scattering Encoded Gold Nanostars for Multiplexed Cell Discrimination. *Chem. Mater.* **2016**, *28*, 6779–6790.

Figures

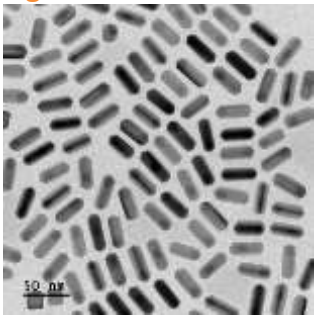

Figure 1. Representative TEM image of the ultrathin silver nanoords.

Biocomposite foams as rapid indicators for pH changes

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Abstract

Herein we present the development and characterization of foams composed of polyvinyl alcohol (PVA), microcrystalline cellulose (CMC) and anthocyanin directly extracted by red cabbage (brassica oleraceae) used as intelligent colorimetric pH indicators. As the physicochemical characterization reveals, the developed foams are highly porous (87%) with pores sizes ranging between 2.06 µm and 5.82 µm, while they absorb efficiently water and moisture. The introduction of the CMC as a filler in the skeleton of the foams results in the decrease of the water and moisture capacity uptake but it significantly increases the speed of the vapors adsorption since it contributes to the increase of the hydrophilicity of the system. Therefore, the biocomposite foams can rapidly change colour upon pH changes of solutions and vapours. In fact, the results for the optical/visual colour changes and UV-visible spectra of the foams revealed that the herein developed biocomposites are universal pH indicators, capable of sensing acidic, neutral or basic environments by displaying a distinct colour for each pH value, few seconds after the exposure (Fig.1). The colour change of the indicators is a simple visual method to detect the pH environment and can be used in various applications [1, 2]. In particular, having in mind that the metabolic products of the bacteria during the food spoilage can produce liquids of different acidity, such biocomposite foams can be used in intelligent food packaging as colorimetric food spoilage indicators [1]. Furthermore, since by monitoring the pH changes one can monitor the cells metabolism, such biocompatible and biodegradable porous pH indicators can be easily implemented in biomedical applications as active scaffolds for tissue growth while simultaneously monitoring the extracellular environment.

References

[1] I. Choi, J. Y. Lee, M. Lacroix and J. Han, Food Chemistry. **218**, 122-128 (2017)Reference 2
[2] K. Devarayan and B. S. Kim, Sensors and Actuators B: Chemical. **209**, 281-286 (2015)

Figures

Figure 1. (a) Anthocyanin solution response upon pH changes (b) Anthocyanin treated PVA/Cellulose foams upon pH changes

POSTERS

Screen-Printed Electroluminescent Lamp Modified with Graphene Oxide as a Sensing Device

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Coupling electrochemical and optical properties are currently opening new possibilities in the sensing field and offering improvements in terms of sensitivity, selectivity, cost effectiveness and ease of use. In this regard herein a screen-printed electroluminescent lamp modified with graphene oxide.[1]The sensor was created using the alternating current electroluminescent (ACEL) technology but modifying its architecture and layers composition with graphene oxide and nafion. The sensing principle is based on the direct relationship between the light intensity of the display and the conductivity of the external layers. The device is able to detect the ionic concentration of any conductive species and can act as humidity sensor. Besides, the response time is so fast that just by coupling the display to a smartphone camera sensor, its potential was expanded for automatically monitoring human breath in real time. This flexible ACEL sensor holds a great potential for future advancement in wearable sensor technology in addition to other applications with interest for diagnostics as well as environmental monitoring, safety and security.

References

[1] Yakoh, A., Álvarez-Diduk, R., Chailapakul, O., & Merkoçi, A. (2018). Screen-Printed Electroluminescent Lamp Modified with Graphene Oxide as a Sensing Device. *ACS applied materials & interfaces*, *10*(24), 20775-20782.
[2]

Figures

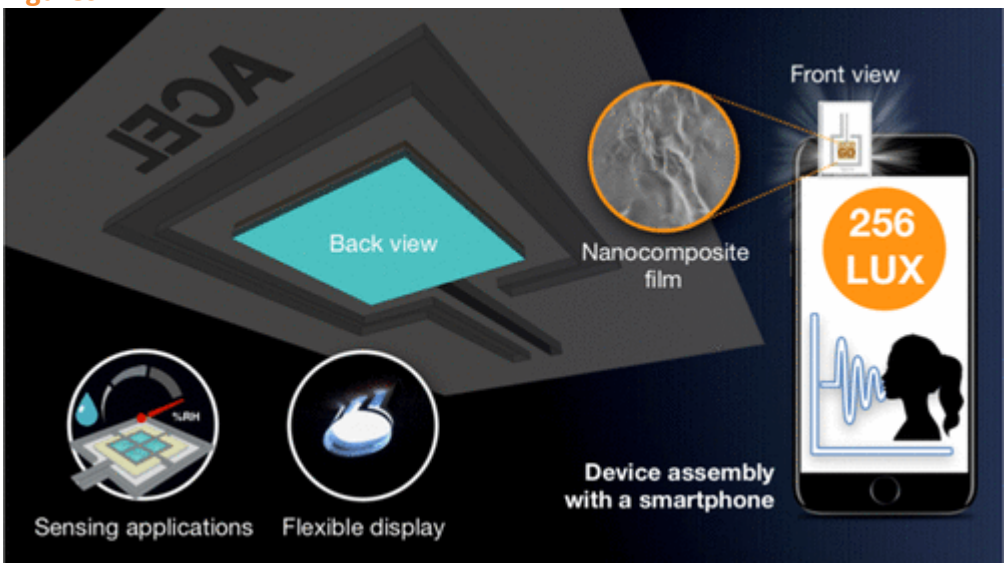

Figure 1.

Mechanical and electrical properties of bio-based PA410/CNT nanocomposites modified with a bio-TPE

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Bio-based polymeric nanocomposites (NCs) were obtained by melt mixing a polyamide 4,10 (PA410) and a thermoplastic elastomer (impact modifier), both commercially available and partially bio-based, with two different commercially available multi-walled carbon nanotubes (CNTs), namely Nanocyl NC7000™ and Plasticyl™ PA 1503 (a masterbatch based on PA6 and Nanocyl NC7000™ CNTs). Mechanical and electrical properties of the resulting NC systems –i.e. PA410/PEBAX/CNT and PA410/PA6/PEBAX/CNT, respectively– were studied. Deformation properties –i.e. ductility and impact resistance– were improved after TPE addition as expected [1], with respect to the unmodified NC systems (Figure 1). A reduction in the percolation concentration (p_c) was also observed in both systems (Figure 2), probably due to a double percolation effect [1, 2].

References

[1] Gonzalez, I., Eguiazabal, J.I., and Nazabal, J. Composites, Part A, 2012. **43**(9): p. 1482-1489.
[2] Sumita, M., et al. Colloid and Polymer Science, 1992. **270**(2): p. 134-139.

Figures

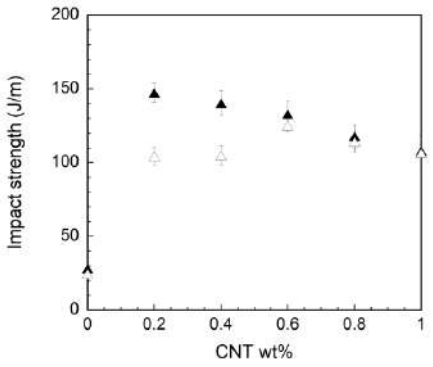

Figure 1. Impact strength of PA410/PEBAX/CNT (open triangles) and PA410/PA6/PEBAX/CNT (filled triangles) NCs.

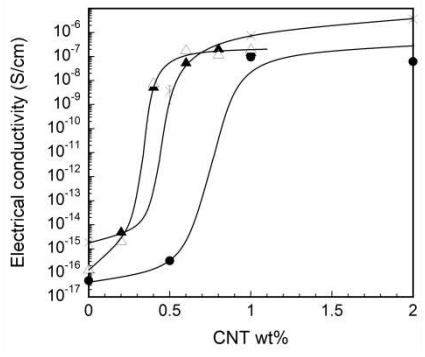

Figure 2. Electrical conductivity of unmodified PA410/CNT (x) and PA410/PA6/CNT (●) and modified PA410/PEBAX/CNT (open triangle) and PA410/PA6/PEBAX/CNT (filled triangle) NCs.

Printed luminescent chemosensor for detection of explosive or explosive-like molecules

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The role of nanoscience in analytical science has been greatly established for the development of chemical sensors with enhanced performance. The design of low-cost, easy-to-fabricate and portable analytical devices with a low limit of detection (LOD), good selectivity, high sensitivity and short response time are in high demand.[1,2,3] In this sense, chemical sensors based on fluorescent quantum dots (QDs) have attracted intense interest because of their excellent optical and electronic properties compared to the routinely employed fluorescent organic dyes.[4] These properties include size-tunable light emission over a wide range of energies, high photoluminescence quantum yield (PL QY), narrow emission line width, and good solution processability.[5] In addition, the physicochemical stability of QDs, their extremely large surface area, as well as the possibility of functionalizing their surface by conjugation with appropriate molecules make them very attractive nanomaterials for ultrasensitive sensors with the possibility of multiplex chemical detection.[6]

In this work, we have developed a novel CdSe QD-polymer-based luminescent chemosensor for the selective detection of explosive or explosive-like molecules. The sensor is based on an array pattern containing either green-emitting or red-emitting CdSe QDs in polycaprolactone (PC) as a polymer host matrix. Here, the sensor fabrication is performed by a microplotter, a direct printing technique based on ultrasonic fluid microdispensing to generate the nanocomposite patterning, resulting in accurate and high-resolution patterns. The transduction mechanism of the sensor is based on changes of the QD photoluminescence (PL) when molecules are adsorbed on the QD surface.

We evaluate the sensing capability of the nanocomposites by exposing the patterns to vapours of some high explosive or explosive-like molecules. Additionally, two different molecules such as 2-mercaptoethanol (MET) and ethylenediamine (EDA) are also tested for comparison. Remarkably, the change in intensity and response times for this two nanocomposites are quite varied depending upon the analyte to which it is exposed. The LOD of the sensors was determined to be as extremely low as 10^{-10} M for all analytes. Monitoring the changes in the fluorescence intensities of both nanocomposite patterns allows to pin-point each analyte on a two-dimensional (2D) map, where selectivity can be greatly enhanced.
We believe that this type of miniaturized luminescent QD-based nanocomposites might form the basis of a fully disposable sensing platform technology to perform effective chemical sensing and detection of many high explosive or explosive-like molecules among others.

References

[1] F. S. Ligler, Anal. Chem., 2009, 81, 519.
[2] R. Abargues, P. J. Rodriguez-Canto, S. Albert, I. Suarez and J. P. Martínez-Pastor, J. Mater. Chem. C, 2014, 2, 908.
[3] P. J. Rodríguez-Cantó, R. Abargues, H. Gordillo, I. Suárez, V. Chirvony, S. Albert, J. Martínez-Pastor, RSC Adv. 2015, 5, 19874
[4] U. Resch-Genger, M. Grabolle, S. Cavaliere-Jaricot, R. Nitschke and T. Nann, Nat. Methods, 2008, 5, 763.

Carbon dots as metal free catalyst for the removal of industrial hazardous dyes

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The discharge of dyes, specifically synthetic dyes into the aqueous system from industrial sources represents a serious environmental problem due to their toxicity to aquatic life and mutagenicity to humans. Some synthetic dyes are extremely resistant to biodegradation and therefore several methods have been developed to assist in their removal [1]. Recently, the use of nanomaterials for the remediation of pollutants has been successfully applied, showing promising results, especially for the removal of dyes from water. As an emerging subset of nanomaterials, carbon dots are nanoparticles in the size range of below 10 nm that present unique characteristics such as stable fluorescence, low toxicity and high aqueous solubility, and are also known to participate in rapid electron transfer properties in catalysis [2]. In this study, carbon dots were synthesised using green precursors (Fig. 1) and tested as metal free catalysts in the "Fenton-like" reaction for the degradation of three synthetic dyes under room temperature (20 ±2°C) and at neutral pH (7.5). Results showed that nanoparticles with 10 nm average diameter were formed and they manifested a negative surface charge across a range of pH conditions. In the presence of H_2O_2, the carbon dots were able to act as catalysts in a "Fenton-like" process removing 100% of dyes (Fig 2) after only 30 minutes; in the absence of carbon dots the removal was of only 15%. The results suggest that the carbon dots are involved in the transference of electrons, participating in the decomposition of H_2O_2, resulting in the generation of free radicals in solution which are responsible for the degradation of dyes.

References

[1] Javaid, R. and U.Y. Qazi, *Catalytic Oxidation Process for the Degradation of Synthetic Dyes: An Overview.* Int J Environ Res Public Health, 2019. **16**(11).
[2] Liu, M.L., et al., *Carbon dots: synthesis, formation mechanism, fluorescence origin and sensing applications.* Green Chemistry, 2019. **21**(3): p. 449-471.

Figures

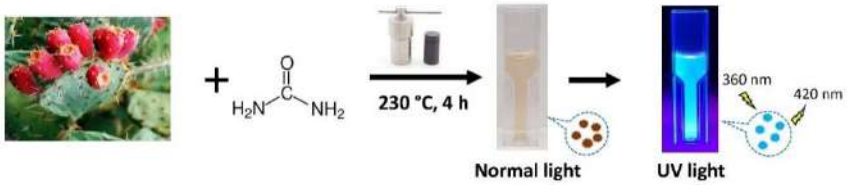

Figure 1. One-pot hydrothermal synthesis of the prickly pear carbon dots.

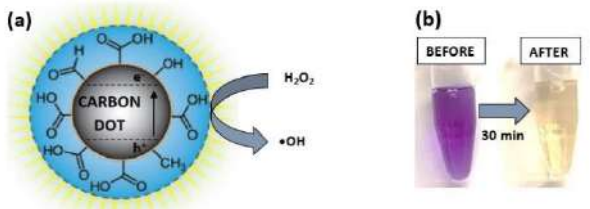

Figure 2. (a) Schematic illustration of the catalytic degradation of dyes (b) digital images of dyes before and after degradation.

Characterization of WTe2 multilayer grown by CVT

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Tungsten ditelluride (WTe_2) is a transition metal dichalcogenides (TMD) [1]. It is considered a 2D material since it shows a multi-layer structure compose by layer W atoms sandwiched between two Te atoms. The layers are implied buy Van der Waals interaction. WTe2 differs from the others TMDs since it present a distorted orthorhombic unit cell where the central W atoms are displaced from the center and form a zig-zag W chain. This distorted crystal and the high SOC made the WTe2 band structure particularity attracting for studying new topological phases. Theoretical studies have predicted that WTe_2 multi-layer could be a type II Weyls semimetal [2]. Whereas a WTe_2 monolayer is a 2D topological insulator at temperature lower (T<100K). ARPES measurements show the opening of a gap [3] and transport studies demonstrate the presence of quantum spin hall effect [4].

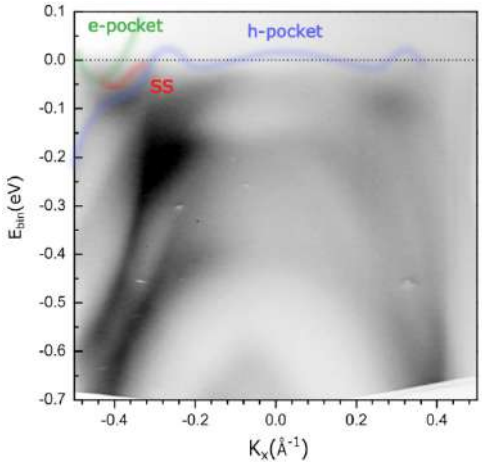

Fig.1 ARPES data along the Γ–Y direction

In this work we present a complete characterization of the crystal and electronic band structure of a multi-layer WTe_2 crystal growth by Chemical Vapor Transport. X-Ray Diffraction and Raman spectroscopy have been used to characterize the crystal structure. Raman spectroscopy has been performed along all the main crystallographic axes showing a high anisotropic behaviour of the scattering peaks. The combination of the two techniques allows us to demonstrate the high crystal structure of our crystals. In-situ exfoliation allowed us to perform X-Ray photoemission spectroscopy (XPS) and angle resolved photoemission spectroscopy (ARPES) on a non-oxidized WTe_2 crystal. XPS measurements confirm the lack of oxidation. The shape, area and position of the XPS peaks allow us to confirm the presence of the expected electrical bounds between W and Te. Our ARPES measurements on the multilayer sample are in accord with the literature and shown the presence of a semimetallic band structure, i.e. the presence of electron and hole pockets. No evidence of type II Weyls semimetal band structure has been found.

Those characterizations allow us to confirm the high quality of our crystals and the possibility to use it in heterostructures with magnetic material and study the proximity effect and the presence of quantum anomalous hall effect.

References

[1] C.-H. Lee, E. C. Silva, L. Calderin, M. A. T. Nguyen, M. J. Hollander, B. Bersch, T. E. Mallouk, and J. A. Robinson, Sci. Rep. 5, 10013 (2015).

[2] A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X.Dai, and B. A. Bernevig, Nature (London) 527, 495 (2015)

[3]] S. Tang et al., Nat. Phys. 13, 683 (2017)

[4] S. Wu, V. Fatemi, Q. D. Gibson, K. Watanabe, T. Taniguchi, R. J. Cava, and P. Jarillo-Herrero, Science 359, 76 (2018)

Structural and electronic properties of molecules adsorption on Blue Phosphorene

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Since the discovery of the two-dimensional (2D) materials such as Graphene, silicene, germanene, etc., with unique optical, electrical, mechanical, transport and gas sensing properties, the interest in the study of these 2D systems has increased significantly. Searching for new alternatives of gas sensing devices, it has been found that one of the most stable allotrope of phosphorus, the black phosphorous or phosphorene, is a good candidate for such applications. Phosphorene is a direct gap semiconductor with an energy gap of the order between 1 and 2 eV, high carrier mobility and armchair ridges [1]. Because of black phosphorene discovery the interest in the study of different allotropes of phosphorus has attracted the attention of the researchers. In addition to black phosphorene, it has been predicted the existence of a second allotrope, the blue phosphorene, which is an indirect gap semiconductor with a gap of the order of 2 eV. This 2D material displays high carrier mobility similar to that of black phosphorus, it has a buckled honeycomb lattice with zigzag ridges [2]. It is important to study blue phosphorene because it displays different electronic, sensing and transport properties in comparison with its counterpart, the black phosphorene.

In this work, the density functional theory (DFT) is applied as implemented in the computational code SIESTA, to investigate molecules adsorption on pristine, Al- doped and a single vacancy blue phosphorene. Five molecules are considered to explore the efficiency and versatility of the blue phosphorene. We want to show that blue phosphorene may be a possible solution of different current problems, such as the environmental pollution and the lack of control getting sub-products in chemical processes that affect the human health. Results show that Al-doped blue phosphorene have stronger interaction energy than pristine and single vacancy blue phosphorene. Single vacancy blue phosphorene has the weakest interaction energy, however it displays magnetic properties. On the other hand, pristine blue phosphorene faces physisorption with no magnetic properties.

References

[1] H. Liu, A. T. Neal, Z. Zhu, Z. Luo, X. Xu, D. Tománek, P. D. Ye, Phosphorene: An Unexplored 2D Semiconductor with a High Hole Mobility, 8, 4, 4033-4041 (2015).
[2] Z. Zhu and D. Tománek, Semiconducting Layered Blue Phosphorus: A Computational Study, Physical Review Letters, 112, 176802 (2014).

Plasmonic nanostructures based hot-electron Si photodetector

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Hot electrons produced from the decay of localized surface plasmons in metallic nanoparticles have been studied in the last year for applications in photodetection and photocatalysis [1]. Hot electron devices consist typically of a metal surface in contact with a semiconductor forming a Schottky barrier [1, 2] and operate based on internal photoemission process (IPE). IPE enables sub-bandgap photodetection making thus silicon devices suitable for operation in NIR-SWIR range.

The paper presents an improved architecture for Au/n-Si Schotky photodetector with plasmonic NPs with high responsivity in the range 1300-1550 nm. To allow incident light to be momentum matched and efficiently coupled to SPs we used nanostructured Ag or Au layers. We developed a simple process for the fabrication of plasmonic nanostructures without using costly and time-consuming nano-lithographic processes. The process is based on vacuum deposition of very thin Ag or Au layer followed by thermal annealing. A periodic structure composed of flattened nano-hemispheres is obtained (fig. 1). The diameter and of the nanostructures depends on the initial thickness of the metal layer and the annealing and can be tuned over a large range (2-2000 nm). The nanostructured layer acts as metamaterial absorber [2] that improves the efficiency of hot electrons generation. The responsivity was further improved by coupling Ag or Au nanoplasmonic nanoparticles with grating-like electrodes. The device spectral characteristics can be tuned by modifying the geometry of the metamaterial.

The experimental devices show very high responsivities, up to 12 mA/W at 1550 nm, and 30 mA/W at 1310 nm @ 5V applied bias, among the highest reported [3].

Acknowledgements: The work was supported by the *IMT core Program MICRO-NANO-SIS PLUS (2019-2022) and the Project EXCEL-IMT, contract No 13PFE 2018-2020.*

References

[1] M. L. Brongersma, N. J. Halas, and P. Nordlander, Nat.Nanotechnol. 10(1), 25–34 (2015).

[2] C. Ng, J. J. Cadusch, S. Dligatch, A. Roberts, T. J. Davis, P.Mulvaney, D. E. Gómez, ACS Nano 2016, 10, 4704−4711.

[3] W. Li, J.Valentine, Nanophotonics 2017; 6(1): 177–191

Figures

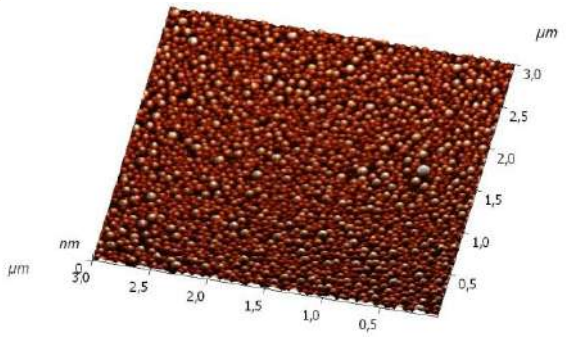

Figure 1. AFM image of Ag NPs obtained by thermal annealing (250 °C, 5') of a150 nm thick Ag layer.

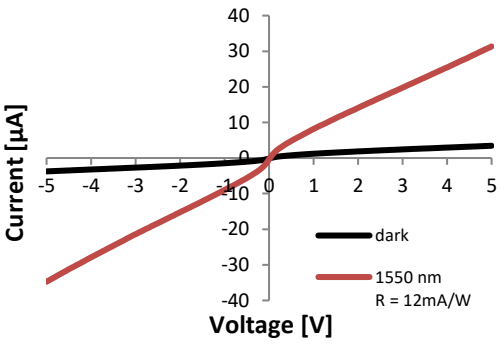

Figure 2. I-V characteristics in dark and under illumination for a Schottky Si device with Au interdigitated electrodes and Ag NPs (ϕ=30 nm).

Molecular dynamics simulation of the interaction between pure and functionalized carbon nanotubes and cement surfaces

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The theoretical study of the properties and structure of cement can be carried out by means of various molecular simulation techniques, among which the molecular dynamics method stand out, since it allows addressing the study of systems that, due to their chemical complexity, must be represented by a large number of atoms

In this work, we present the results of molecular dynamics simulation of the interaction between pure or functionalized single-walled carbon nanotubes (SWCNTs) or multiwalled carbon nanotubes (MWCNTs) and a representative cement surface (figure 1). The goal is to study the influence of the functionalization type of the CNTs on the interaction between the cement and CNTs, in order to reinforce this interaction, achieve a good CNTs dispersion and improve the mechanical properties of the cement, as well as analyze the differences obtained between SWCNTs and MWCNT.

Figures

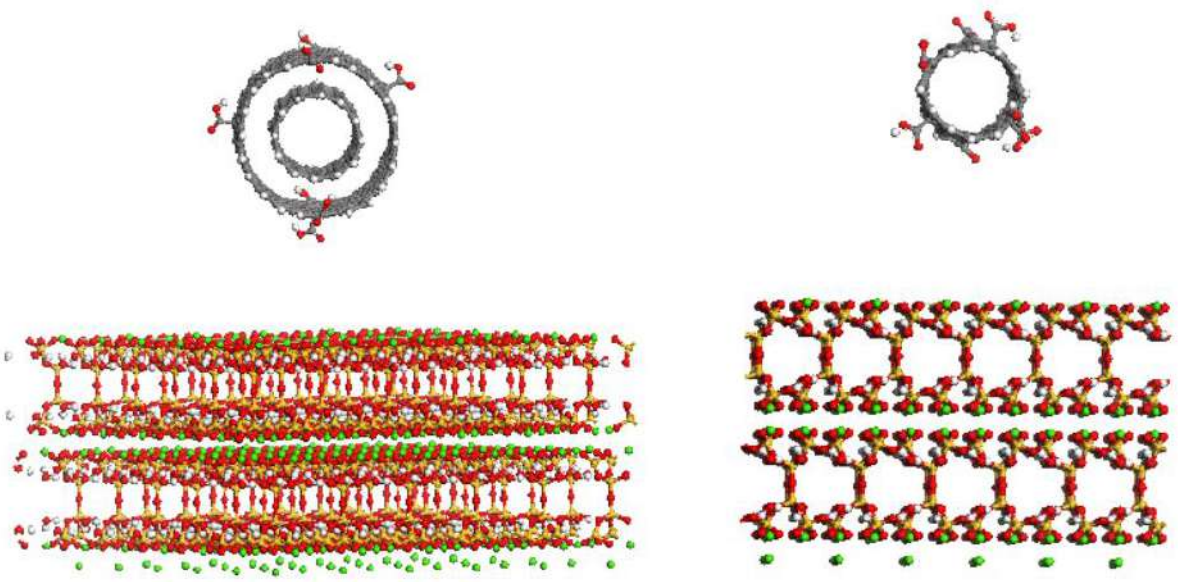

Figure 1. Two examples of functionalized carbon nanotubes interacting with the cement surface

Effect of pH on Electrodeposited CZTS Thin Films on ITO Substrates

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Abstract

In this study, Cu2ZnSnS4 (CZTS) thin films were deposited on ITO substrates by using single step electrodeposition method. CZTS absorber layers have been tried to be obtained at four different pH values of 4.70, 5.10, 5.70 and 6.23 which are commonly used in literature. Trisodium citrate was used as a complexing agent for co-electrodeposition. CZTS thin films annealed for recrystallize in stoichiometric kesterite structure after deposition at 580 °C in sulfur powder and N2 atmosphere for 60 min. It is clear that a highquality film can be obtained in cathodic potential with -1.1 V and deposition time with 2700 seconds, pH value with 5.7 at room temperature respectively. The structural, morphological and optical properties of CZTS thin films have been investigated by using X-ray diffraction (XRD), optical absorption techniques, scanning electron microscopy (SEM), atomic force microscopy (AFM) and Raman spectroscopy measurements, respectively. This indicates that quaternary co-electrodeposition method is a very convenient process for growth of CZTS films for the application in photovoltaic devices.

A first principles exploration of Charge Density Waves in 2D Transition Metal Dichalcogenides

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We explore by means of Density Functional Theory the electronic structure and the manifestation of Charge Density Wave (CDWs) in three different single-layered transition metal dichalcogenides: $TiSe_2$, $TiTe_2$ and $NbSe_2$. Each of these materials presents a particularity from the viewpoint of behavioral spectra of 2D materials in the CDW phase.

In the case of $TiSe_2$ we show that the prevailing stable phase of the CDW arises from the combination of the phonon modes coming from the three inequivalent M points[1]. The effect of charge doping on $TiSe_2$ single-layers indicates a suppression of the CDW phase for large enough values of both electrons, respectively doping.

$NbSe_2$ single-layers present an unexpected CDW phase where up to six different 3x3 modulations could be stabilized. From these six structures, three of them are experimentally found to coexist. In opposition with $TiSe_2$, $NbSe_2$ shows a persistence of the CDW phase with doping with both electrons and holes[3].

Finally, for the case of $TiTe_2$ we suggest that tensile bi-axial strain could stabilize the CDW phase starting from the single-layer configuration and going up to several layers[2].

Acknowledgements: This work was supported by Spanish MICIU, AEI and EU FEDER (Grant No. PGC2018-096955-B-C4). ICN2 and ICMAB are supported by the Spanish MICIU and AEI Severo Ochoa Centers of Excellence Program (Grants No. SEV-2017-0706 and No. SEV-2015-0496), and ICN2 by Generalitat de Catalunya (CERCA Programme).

References

[1] B. Guster, E. Canadell, M. Pruneda and P. Ordejón, 2D Materials 5 025024 (2018)
[2] B. Guster, R. Robles, M. Pruneda, E. Canadell and P. Ordejón, 2D Materials 6 015027 (2019)
[3] B. Guster, C. Rubio-Verdú, R. Robles, J. Zaldívar, P. Dreher, M. Pruneda, J. A. Silva-Guillén, D.-J. Choi, J. I. Pascual, M. M. Ugeda, P. Ordejón, and E. Canadell, Nano Letters 19, 3027 (2019)

A single layer self-assembled radiative cooler

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Phonons, the quasi-particles that carry heat and sound, are practically involved in all kind of mechanical, optical, and thermal phenomena. By micro or nano-structuring a surface, phonons can be engineered to make them interact resonantly with photons and achieve interesting effects such as radiative cooling, which involves decreasing the temperature of a body without using electricity or any other kind of extra energy input. Radiative cooling has gained attention recently, because modern cooling technologies are particularly energy-consuming and a ten-fold grow in the energy demand associated to them is expected in the next 30 years, due to global warming. To address this global challenge, we propose a thermo-functional material that is capable of removing heat passively from devices or surfaces that undergo critical heating during operation. Our solution is based on a self-assembled single-layer array of SiO2 microspheres on a soda-lime slab. The working principle of the proposed cooling device is based on the interaction of the transverse optical phonons and equally polarized electromagnetic waves, which results in an intense evanescent field confined at the surface of a polar-dielectric interface. Such surface excitations, so called surface phonon polaritons (SPhP), have the ability to enhance thermal energy conduction [1], and, in the presence of a grating, they can be diffracted to the far-field as infrared thermal energy [2]. Thus, we engineer the thermo-optical properties of our device to remove heat and evacuate it through the transparent infrared atmospheric window, as infrared thermal energy to then deposit it into the outer space at 3K which acts as a heat sink. In this work, we will present how the temperature of a crystalline silicon wafer is lowered during daytime when the self-assembled single-layer cooler is placed on its surface, providing experimental evidence of above-ambient daytime radiative cooling.

References

[1] Tervo, E. J., Adewuyi, O. S., Hammonds, J. S. & Cola, B. A. High thermal conductivity in polaritonic SiO_2 nanoparticle beds. Mater. Horiz. 3, 434–441 ,2016.
[2] Joulain, K., Mulet, J.-P., Marquier, F., Carminati, R. and Greffet, J.-J. Surface electromagnetic waves thermally excited: Radiative heat transfer, coherence properties and Casimir forces revisited in the near field. Surf. Sci. Rep. 57, 59112 ,2005

Symmetry protection of N-photon angular momentum states when interacting with cylindrical systems

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In the interaction with a cylindrical sample, the z-component of the total angular momentum of light, m, is a conserved quantity, whereas other quantum numbers are not (as λ, the quantum number related to helicity). Importantly, this helicity-angular momentum framework has recently allowed the study of quantum light matter interactions in nanoholes, for N = 2 and considering states with $m = 0$ [1].

In this work we show a generalization of this construction for N-photon states employing single photons with both $m = 0$ and also $m \neq 0$. Moreover, we find that N-photon symmetry protected states, that is states that are protected in the interaction with any cylindrical scatterer, can be constructed in a very general way.

Finally, we show examples of symmetry protected 2 and 3-photon states that can be found using input modes with $m \neq 0$, even when the input photons are in different modes with different angular momenta.

References

[1] A. Büse et al. Symmetry Protection of Photonic Entanglement in the Interaction with a Single Nanoaperture. Phys. Rev. Lett. 121, 173901 (2018).

Benchmarking Starting-Points of the G_0W_0 for Open-Shell Molecules

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Hedin's GW approximation (GWA) has gained popularity in the material science community because of its high quality and relatively low computational cost. A prerequisite to describe magnetic materials is the capability to describe systems containing unpaired electrons. In this study, we benchmark the ionization energy calculated by G_0W_0 on top of different unrestricted starting-points for small open-shell molecules using Dunning's correlation-consistent basis sets expanded in terms of Gaussian functions. As an alternative route, electron affinity of the positively charged molecules are calculated as well. Results are carefully compared with a variety of correlated methods including CCSD(T).
It is revealed that G_0W_0 provides a systematic and accurate method to compute the quasi-particle energy levels of such molecules with convincing evidence of reliability similar to the case of closed-shell molecules. Furthermore, GWA provides a correct ordering of the molecular orbitals based upon orbital energy eigenvalues in consistent agreement with the Dyson orbitals. The present implementation of GWA is based on the use of basis sets of atomic orbitals and provides a good compromise between accuracy and computational expense, suitable to be applied to study magnetic materials.

Figure

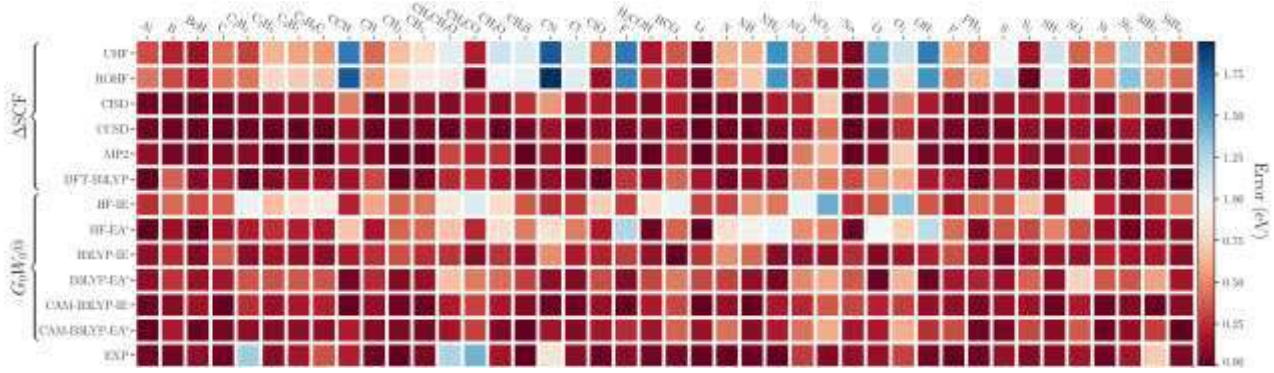

Figure 1. Heatmap presentation of errors in eV obtained from the various methods using a cc-pVQZ basis with respect to the ΔSCF-CCSD(T) total energy difference. G_0W_0 results were calculated by two ways: IE of neutral molecule and EA of the molecule's cation (EA^+).

Laser Induced Graphene Flexible In-Plane Microsupercapacitors

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The continuous miniaturization of electronics and energy storage devices are facilitating the increase of wearable devices and sensors. Flexible micro-supercapacitors (MSCs) are a promising and low cost power source for this devices, because compared with microbatteries, which are the used solution nowadays, MSCs presents faster charge/discharge rate, higher power density and higher cyclability [1]. In this study, a flexible, in-plane micro-supercapacitor with interdigitated electrodes has been fabricated. A commercial polyimide film has been used as the substrate, and converted to laser induced graphene (LIG) by direct laser irradiation with a CO_2 infrared laser. This LIG is a porous 3D material that exhibits high surface area, high thermal and chemical stability and good conductivity [2], so it presents huge potential for electrochemical and energy storage applications. In order to improve the capacitance of the device, cobalt based nanostructures have been deposited onto the LIG by electrochemical deposition. Finally, in order to avoid costly encapsulation processes and possible leakages, a solid gel electrolyte have been used.

References

[1] Li, L., et al. Advanced Materials, 2016. v. 28, p. 838-845.
[2] Ye, R., James, D.K. and Tour, J.M. Advanced Materials, 2019, v. 31, 1803621

Figures

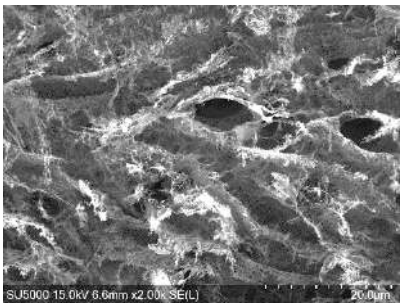

Figure 1. SEM image of the obtained Laser Induced Graphene.

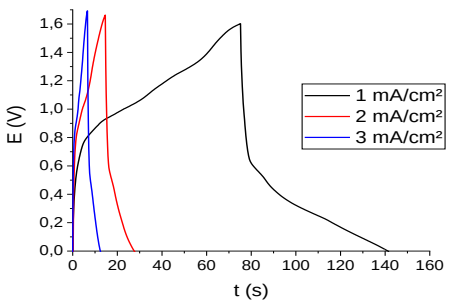

Figure 2. CC curves of LIG-MSCs at different current densities.

STRONG CORRELATION IN ONE- AND TWO-DIMENSIONAL SYSTEMS

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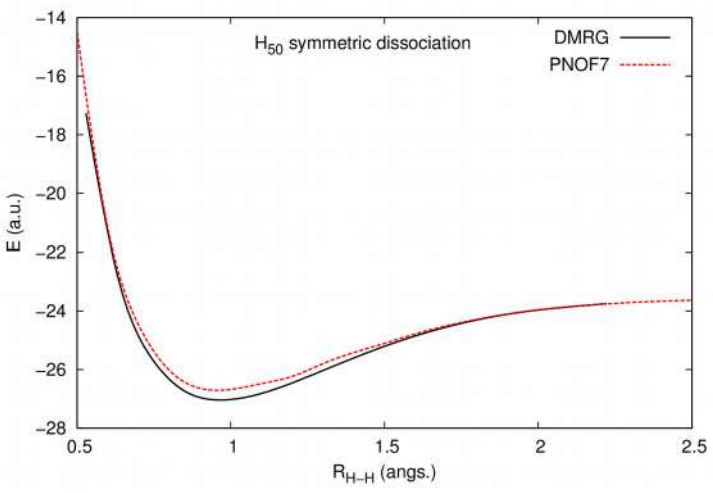
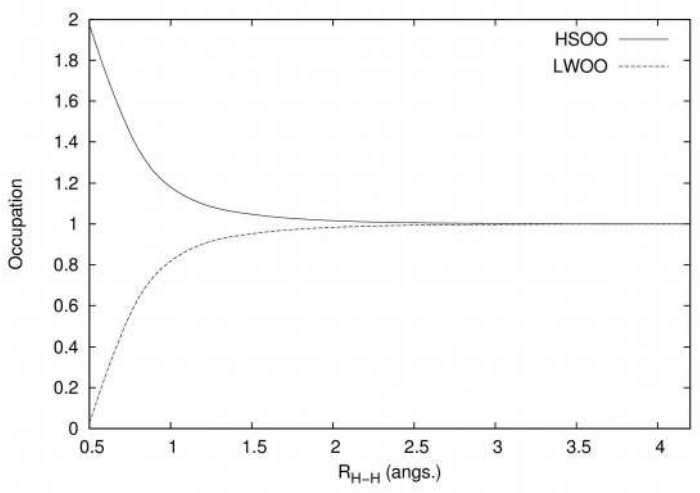
DFT fails dramatically to describe strongly correlated electrons [1]. Natural Orbital Functional (NOF) theory is an ideal alternative to study strongly correlated electrons within one-particle theories. We show the ability of the PNOF7 approximation [2,3] to describe static correlation effects in two-dimensional systems. Correlation energies obtained by using PNOF7 are comparable to those of exact diagonalization, density matrix renormalization group, and auxiliary-field quantum Monte Carlo calculations for the two-dimensional Hubbard model up to 144 electrons, which is considered the prototype to study high-temperature superconductors [4].For the latter, accurate results are obtained when particle-hole symmetry is broken away from half-filling. We report energies for different spin multiplicities of the Hubbard and the quantum mechanical Hamiltonians by means of an approximation exempt of spin contamination effects [5]. Dissociation processes are studied in one- and two-dimensional hydrogen lattices.

References

[1] J. Phys.: Condens. Matter,vol. 27, no. 39, p. 393001, 2015
[2] Eur. Phys. J. B, vol. 91, p. 109, 2018
[3] Phys. Rev. Lett., vol. 119, pp. 063 002#5, 2017
[4] Science, vol. 358, no. 6367, pp. 1155#1160, 2017
[5] arXiv:1908.05501 [physics.chem-ph] (accepted in PRA)

Figures





Symmetry protection of N-photon angular momentum states when interacting with cylindrical systems

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In the interaction with a cylindrical sample, the z-component of the total angular momentum of light, m, is a conserved quantity, whereas other quantum numbers are not (as λ, the quantum number related to helicity). Importantly, this helicity-angular momentum framework has recently allowed the study of quantum light matter interactions in nanoholes, for N = 2 and considering states with $m = 0$ [1].

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References

[1] A. Büse et al. Symmetry Protection of Photonic Entanglement in the Interaction with a Single Nanoaperture. Phys. Rev. Lett. 121, 173901 (2018).

Asymmetry and spin-orbit coupling of light scattered from subwavelength particles

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Light spin-orbit angular momentum (AM) coupling phenomena are receiving an increasing interest in the analysis of scattering processes from sub-wavelength objects [1]. They are of particular relevance in far-field optical imaging [2], where this coupling leads to significant shifts between the measured and actual position of particles [3], known as optical mirages for spherical scatterers [4]. Here we show that for small isotropic particles with electric and magnetic dipolar response, the angular scattering pattern of the spin-orbit coupling and optical mirage is fully determined by the (measurable) degree of circular polarization (DoCP) at a right-angle scattering [5]. We explicitly show that the maximum AM exchange, the zeros of the DoCP and the maximum optical mirage do not appear at the same scattering angle. Our results open the possibility to infer optical properties by a single measurement of the polarization in the far-field limit.

References

[1] H. He, M. Friese, N. Heckenberg, and H. Rubinsztein-Dunlop, Phys. Rev. Lett. 75, 826 (1995).
[2] J. H. Crichton and P. L. Marston, Electron. J. Differ. Equations 4, 37 (2000).
[3] D. Haefner, S. Sukhov, and A. Dogariu, Phys. Lett. 102, 123903 (2009).
[4] Olmos-Trigo, J., Sanz-Fernández, C., García-Etxarri, A., Molina-Terriza, G., Bergeret, F. S., & Sáenz, J. J. Phys. Rev. A , 99 (1), 013852 (2019).
[5] I. Fernandez-Corbaton, X. Zambrana-Puyalto, and G. Molina-Terriza, Phys. Rev. A 86, 042103 (2012).

Effect of CNT dispersion and aspect ratio on mechanical and electrical properties of bio-based PA410/CNT nanocomposites

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Bio-based polymeric nanocomposites (NCs) were obtained by melt mixing a partially bio-based commercial polyamide 4,10 (PA410) with three different commercially available multi-walled carbon nanotubes (CNTs), namely Cheap Tubes 20-30, Nanocyl NC7000™ and Plasticyl™ PA 1503 (a masterbatch based on PA6 and Nanocyl NC7000™ CNTs). Mechanical and electrical properties of the resulting NC systems –i.e. PA410/CNT(1), PA410/CNT(2) and PA410/PA6/CNT, respectively– were studied. A considerably lower percolation concentration (p_c) (Figure 1), together with improved rigidity (Figure 2), was achieved with the addition of Nanocyl NC7000™ CNTs, both in the form of powder and masterbatch, in comparison to Cheap Tubes CNTs. The superior electrical and mechanical performance of these NCs was eventually atributted to the better dispersion level and the higher aspect ratio observed for Nanocyl NC7000™ nanotubes [1, 2].

References

[1] Haggenmueller, R., et al. Polymer, 2006. **47**(7): p. 2381-2388.
[2] Krause, B., Potschke, P., and Haeussler, L. Compos. Sci. Technol., 2009. **69**(10): p. 1505-1515.

Figures

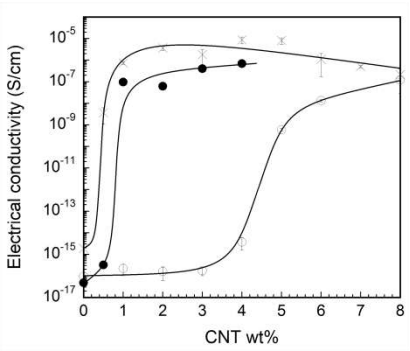

Figure 1. Electrical conductivity of PA410/CNT(1) NCs (○), PA410/CNT(2) NCs (x) and PA410/PA6/CNT NCs(●).

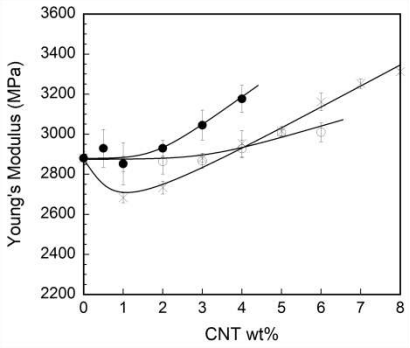

Figure 2. Young's modulus of PA410/CNT(1) NCs (○), PA410/CNT(2) NCs (x) and PA410/PA6/CNT NCs(●).

Correlating atomic scale structure and activity of model catalysts for Oxygen Evolution Reaction

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Water splitting into hydrogen and oxygen is a clean, sustainable and fossil-free route to production of hydrogen gas, the ultimate clean energy carrier (figure 1). The oxygen evolution reaction (OER) is considered the limiting half-reaction in the overall process, due to its complex kinetics and large overpotential [1]. To develop new materials with optimized catalytic properties is one of the most crucial challenges towards a more sustainable way of clean and renewable energy sources. In order to achieve this long-standing goal, atomistic understanding of the processes taking place at the electrode-electrolyte interface is demanded. Here we provide structural, chemical and electrochemical characterization on exactly the same sample. Our customized experimental set up allows for transferring the catalyst from ultra high vacuum (UHV) conditions to an electrochemical cell in a controlled atmosphere. This optimized approach enables the direct correlation between the surface properties at the microscopic scale, -composition and structure-, and the macroscopic response of the catalyst.

Ruthenium oxides are promising earth-abundant catalysts for the OER in both, alkaline and acidic electrolyte. We explore different oxidation states of Ru surfaces, grown using two different methodologies under UHV conditions: direct oxidation of the metallic surface and molecular beam epitaxy of thin films of the oxide [2]. In situ structural and chemical characterization of the prepared Ru-oxides are carried out by Low Energy Electron Diffraction (LEED) and X-Ray Photoemission spectroscopy (XPS). The oxide surfaces previously characterized under UHV conditions are then transferred under controlled atmospheric conditions into the electrochemical cell for the electrochemical test. After the electrochemical measurements, the sample is transferred back to the UHV system in order to identify potential changes induced by the electrochemical process.

References

[1] N. B. Halck, V. Petrykin, P. Krtil, and J. Rossmeisl, *Phys. Chem. Chem. Phys.*, **16**(27),13682–13688 (2014)
[2] B. Herd, J. C. Goritzka, and H. Over, *J. Phys. Chem,* **117**, 15148-15154 (2013)

Figures

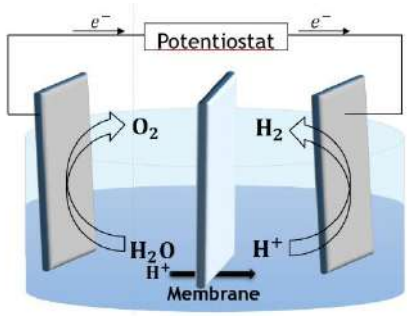

Figure 1. Scheme of an electrochemical cell with hydrogen evolution reaction and oxygen evolution reaction.

In-Situ characterization of the thermal and elastic behavior of rectifier diodes under working conditions

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A widely extended application in semiconductor-based technology is the use of rectifier diodes in vehicles alternators to convert part of the mechanical energy into electrical energy[1]. The most common failures in electric alternators are due to the electrochemical corrosion of the diodes or to damages as a consequence of the high current that circulates through diodes, which causes a significant temperature increase[2]. This temperature increase is one of the system weakness, affecting directly to the device operation parameters. The multicomponent nature of diodes, which are built up by different materials (epoxies, metals and semiconductors) with different physical characteristics and, therefore, with different behavior, is responsible of the appearance of diverse damaging phenomena such as the mechanical stress generation in the device.

This work shows the structural, compositional and physical characteristics of several diodes, currently used in automotive alternators. A study of the diodes has been carried out under certain working conditions which can lead to system failures, as well as to some phenomena allowing to understand their working mode. Some techniques such as confocal Raman microscopy and infrared thermography have allowed an *in operando* study of the diodes in forward biased and reverse biased conditions. The results show the device behavior at the interfaces, the generated stress in the different components and some system failure modes.

References

(1) Rahimian, M. M.; Toliyat, H. A.; Lipo, T. A. A Comprehensive Analysis of a Locomotive Traction System Including Main Alternator, Bridge Rectifiers, Contactor, and DC Traction Motors. **2002**, 118–124.

(2) Ayadi, M.; Ghariani, M.; Toumi, A. Rectifier Dynamic Electro-Thermal Simulation for Power Factor Correction in Electric Vehicles Application. *J. Electr. Eng. Technol.* **2016**, *11* (5), 1153–1164.

Figures

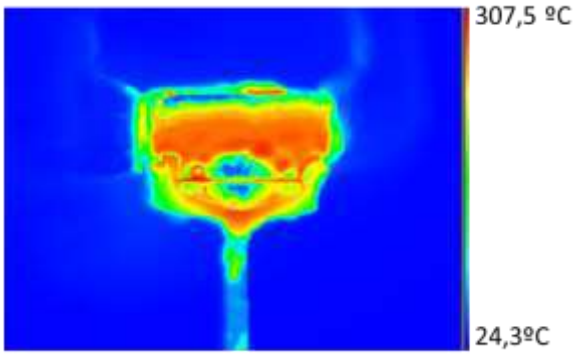

Figure 1. Thermograph of one cut diode after breakdown at reverse polarization.

Spin-dependent Electron Transfer Dynamics at a Model Interface: Key Role of Bandstructure

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We investigate theoretically the charge transfer dynamics of core-excited Ar on Co(001) and Fe(110). For these systems, recent core-hole-clock measurements [1] of the lifetime of the photo-excited 4s level of Ar* have shown a clear dependence on the spin of the excited electron. Minority electrons in the Ar* 4s resonance decay significantly faster than majority electrons. We investigate such processes using Green's functions techniques on top of semi-local density functional theory (DFT) calculations, explicitly including the effect of the coupling to the semi-infinite substrate [2, 3]. Our calculations agree with the observed behavior and allow analyzing in detail the origin of this phenomenon [4]. To gain a better understanding we have performed a detailed analysis of the energy and distance dependency of the substrate-adsorbate coupling. We have also considered different descriptions of the, inherently ill-defined, wave-packet describing the initial state of the photo-excited electron. The key ingredient behind the observed behavior is the spin-dependence of the bandstructure of the substrate and, in particular, the very different position of the Ar* 4s level within the projected band gap appearing around Gamma in the dispersive bands of Co(001) and Fe(110) for both spin channels.

References

[1] F. Blobner, et al., Phys. Rev. Lett. 112, 086801 (2014)
[2] D. Sánchez-Portal, Prog. Surf. Sci. 82, 313–335 (2007)
[3] M. Müller, et al., J. Phys. Chem. C 122, 7575-7585 (2018)
[4] M. Müller, PhD thesis dissertation; M. Müller, P. M. Echenique, D. Sánchez-Portal, in preparation

Figures

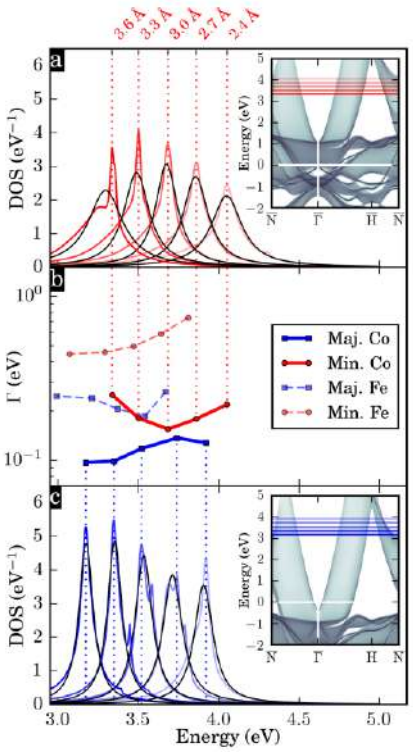

Figure 1. Computed first resonance above the Fermi level for Ar*($2p^{-1}4s$) on Co(0001) for adsorption distances ranging from 2.4 to 3.6 Å in the minority (a) and majority spin channel (c). Different shadings of the colored lines in the plots encode the adsorption heights. The energy positions of the resonance maxima are marked by horizontal lines with respect to the band structure of the Co(0001) surface in the insets, and strongly overlap with the region covered by band gaps around the Γ-point. Panel (b) collects the linewidths Γ(eV) of the Ar* resonances according to a Lorentzian fitting of the peaks (black lines) in (a, c). The spin-dependent linewidths of similar Ar*-resonances on Fe(110) are also shown in (b).

Non-local magnetolectric effects in diffusive conductors with spatially inhomogeneous spin-orbit coupling

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We present a theoretical study of non-local magnetoelectric effects [1] in diffusive hybrid structures with an intrinsic linear-in-momentum spin-orbit coupling (SOC) which is assumed to be spatially inhomogeneous. Our analysis is based on the SU(2)-covariant drift-diffusion equations [2,3] from which we derive the BC at hybrid interfaces. Within this formulation, the spin current is covariantly conserved when the spin relaxation is only due to the intrinsic SOC. This conservation leads to the absence of spin Hall (SH) [1] currents in homogeneous systems. We also consider extrinsic sources of relaxation (ESR), as magnetic impurities, which break the covariant spin conservation, and may lead to SH currents. We apply our model to describe non-local transport in a system with an interface separating two regions: one normal region without intrinsic SOC and one with a Rashba SOC. We first explore the inverse spin-galvanic effect, i.e., a spin polarization induced by an electric field [4,5]. We demonstrate how the spatial behavior of such spin density depends on both, the direction of the electric field and the strength of the ESR rate. We also study the spin-to-charge conversion [6], and compute the charge current and the distribution of electrochemical potential in the Rashba region induced by a spin current injected into the normal region. In systems with an inhomogeneous SOC varying in one spatial direction, we find an interesting non-local reciprocity between the spin density induced by a charge current at a given point in space, and the spatially integrated current induced by a spin density injected at the same point.

References

[1] J. Sinova, S. O. Valenzuela, J. Wunderlich, C. H. Back, and T. Jungwirth, Reviews of Modern Physics 87, 1213 (2015).
[2] J. E. Hirsch, Physical Review Letters 83, 1834 (1999).
[3] C. Gorini, P. Schwab, R. Raimondi, and A. L. Shelankov, Physical Review B 82, 195316 (2010).
[4] V. M. Edelstein, Solid State Communications 73, 233 (1990).
[5] M. I. Dyakonov and V. I. Perel, Physics Letters A 35, 459 (1971).
[6] E. G. Mishchenko, A. V. Shytov, and B. I. Halperin, Physical review letters 93, 226602 (2004).

Novel α-fetoprotein (AFP) third domain-conjugated PLGA nanoparticles with paclitaxel: pharmacokinetics and biodistribution study

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Intoduction

Paclitaxel (PTX) is a highly hydrophobic anticancer drug, therefore cremophor EL solution is applied for its clinical administration, which causes serious allergic reactions to the subjects after intravenous use [1]. Moreover, PTX implementation is limited due to non-specific distribution throughout the body; toxicity to healthy tissues, limiting the dose and frequency of the treatment. Drug encapsulation into PLGA nanoparticles (NPS) conjugated with vector molecule is a well-known strategy, allowing to rich its active targeted delivery and to enhance its bioavailability [2]. Thus, we developed a novel PTX PLGA nanoparticles conjugated with recombinant α-fetoprotein third domain (rAFP3d-NPs), which is known as a tumor-specific biomarker [3].

Methods

In pharmacokinetics experiments 180 female Wistar rats were randomly divided into three groups, each group being received 6 mg/kg of paclitaxel injection through tail vein in the form of rAFP3d-NPs or PTX cremophor EL solution. At certain time points after dosing, blood samples were collected and organs were harvested followed by extraction and HPLC analysis.

Results

Favorable chromatography conditions allowing the baseline separation of the analyte with the internal standard and other exogenous materials were developed and the HPLC method was validated. All the PTX formulations demonstrated a gradual declining trend after reaching maximum of the concentrations. Pharmacokinetics parameters such as $AUC_{(0-\infty)}$ and $t_{1/2}$ were 3 times higher for rAFP3d-NPs with low clearance rate, compared with PTX cremophor EL solution, indicating longer retention of PTX in systemic circulation. In addition, accumulation of rAFP3d-NPs was predominantly observed in liver and spleen over a period of 12 hours.

Conclusion

A simple and effective HPLC method was provided for the determination of rAFP3d-NPs in rats with good accuracy and precision. Novel PTX delivery system demonstrated prolonged release profile, when compared with PTX cremophor EL solution. Our findings indicate an increase in PTX bioavailability and pharmacokinetics profile improvement and also are the basis for determining the optimal dosing regimen in rAFP3d-NPs further studies on immunodeficiency models *in vivo*.

References

[1] Xiao K. et al. A self-assembling nanoparticle for paclitaxel delivery in ovarian cancer //Biomaterials. – 2009. – V. 30. – №. 30. – P. 6006-6016.
[2] Senapati S. et al. Controlled drug delivery vehicles for cancer treatment and their performance //Signal transduction and targeted therapy. – 2018. – V. 3. – №. 1. – P. 7.
[3] Naz Z. et al. Alpha-fetoprotein: A fabulous biomarker in hepatocellular, gastric and rectal cancer diagnosis //Biomedical Research. – 2018. – V. 29. – №. 12. – P. 2478-2483.

Taylor-Aris dispersion Analysis to characterise Plasmonic Nanoparticles

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The wide range of nanoparticles of different composition, size, and shape developed on demand requires a full and reliable characterization of their physicochemical properties.[1] In this context, UV-Vis spectroscopy, light scattering, and electron microscopy are the most commonly used techniques. However, each technique has its inherent limitations and strengths. In this regard, it is necessary to develop new techniques that either overcome the limitations of the existing techniques or can be used in combination with them to verify the obtained results. Taylor-Aris dispersion analysis (TDA) is an absolute technique initially developed to determine the apparent size of proteins and polymeric particles.[2] Recently, it has been demonstrated that silica nanoparticles and superparamagnetic particles can be successfully characterized by TDA.[3][4] Relying on the fact that detection by TDA is based on absorption, herein we demonstrate that the size of spherical and anisotropic metallic nanoparticles can be determined by TDA. In order to prove the versatility of the technique, we also analyzed gold-silver mixtures. Results were compared with data obtained by polarized and depolarized light scattering (DLS and DDLS) and transmission electron microscopy (TEM).

References

[1] S. Mourdikoudis, R. M. Pallares, N. T. K. Thanh, *Nanoscale* **2018**, *10*, 12871.
[2] A. Hawe, W. L. Hulse, W. Jiskoot, R. T. Forbes, *Pharm. Res.* **2011**, *28*, 2302.
[3] D. A. Urban, A. M. Milosevic, D. Bossert, F. Crippa, T. L. Moore, C. Geers, S. Balog, B. Rothen-Rutishauser, A. Petri-Fink, *Colloid Interface Sci. Commun.* **2018**, *22*, 29.
[4] U. Pyell, A. H. Jalil, D. A. Urban, C. Pfeiffer, B. Pelaz, W. J. Parak, *J. Colloid Interface Sci.* **2015**, *457*, 131.

In-lab Micro XRF at high lateral resolution

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Abstract

XRF (X-ray Fluorescence) is a powerful technique for elemental analysis. The lateral resolution is given by the excitation beam diameter in classical XRF configuration or by the characteristics of the optics used for fluorescence signal collection in the case of confocal XRF. We have developed a software to estimate the ultimate lateral resolution which could be reached in XRF analysis as a function of source brightness by calculation of the collected signal magnitude. These calculations are based on the finite element method. To check the simulation data pertinence, we have developed an XRF test-bed using an Rh-target low power source (figure 1). A polycapillary lens is used to tightly focus the primary beam and the sample X-ray fluorescence is collected through a cylindrical capillary [1]. Both capillaries are positioned in a confocal type configuration. The influence of the capillary radius, length and working distance on the fluorescence signal magnitude collection is investigated. Simulations allow to predict the ultimate limit of the technique in terms of lateral resolution. Further measurements replacing cylindrical capillary by elliptical capillaries are presented.

References

[1] M. Dehlinger, C. Fauquet, S. Lavandier, O. Aumporn, F. Jandard, V. Arkadiev, A. Bjeoumikhov and D. Tonneau, Nanoscale Research Letters 2013, 8:271

Figures

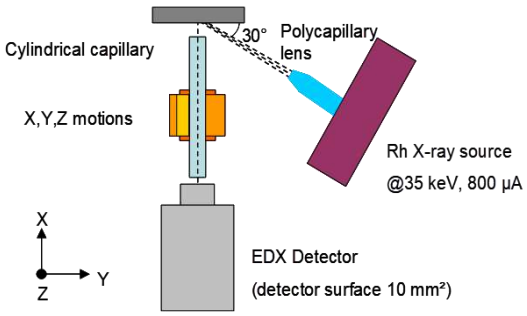

Figure 1. Test bed for simulation results validation

On-surface Boroxine synthesis: from 1D to 2D nanostructures

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Boronic acids represent a powerful tool for the construction of nano-architectures. The reversible interactions that boronic acids can take part in can be used in many fields like self-assembly, self-healing materials, sensing and chemical synthesis [1]. In the present work we have characterized the on-surface synthesis of boroxine based nanostructures on the Au (111) surface, using the naphthyl boronic acid (NBA) as precursor. XPS, NEXAFS and STM measurements gave us a clear view of the chemistry and morphology of the molecular assemblies as a function of the substrate temperature. This study revealed that increasing the sample temperature different synthesis process are activated, which lead to the formation of molecules with increasing size and different chemical properties (figure 2). The main reaction we observe, that occurs already at RT, is the condensation of the boronic terminations and the formation of boroxinated trimers (TNB in figure 1). An interesting feature of the condensation reaction which leads to boroxine (B_3O_3) rings is that it is fast and reversible, indeed B-O covalent bonds can be formed and broken reversibly under equilibrium control. This opens the possibility of constructing molecular architectures with reversible structural elements.

Furthermore, increasing the sample temperature boroxine rings tend to form covalent bonds with nearby boroxines giving rise to more extended molecular assemblies (Figure 2). The dynamic nature of B-O covalent bonds allows to build robust nanostructures whose dimensions and electronic properties are tuned simply varying the sample temperature. In addition to the structural function of boroxine rings, our research group has recently shown many interesting electronic properties of boroxines and the possibility to create a 2D material entirely made up of boroxine rings [2][3].

References

[1] Andrew L. Korich and Peter M. Iovine. Boroxine chemistry and applications: A perspective. *The Royal Society of Chemistry, 39:1423-1431, 2010*

[2] Toffoli et al., *Chem. Science*., 2017, 8, 3789-3798

[3] Stredansky et al., *Chem. Communication*, 2018

Figures

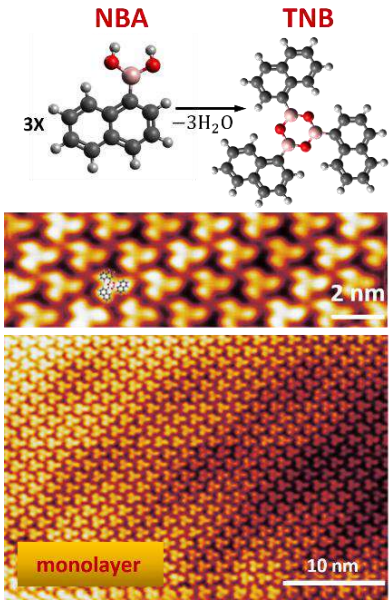

Figure 1. Experimental STM images after NBA deposition at 330 K. The whole surface is covered by clover like structures, i.e. Tri-Naphthyl Boroxine molecules.

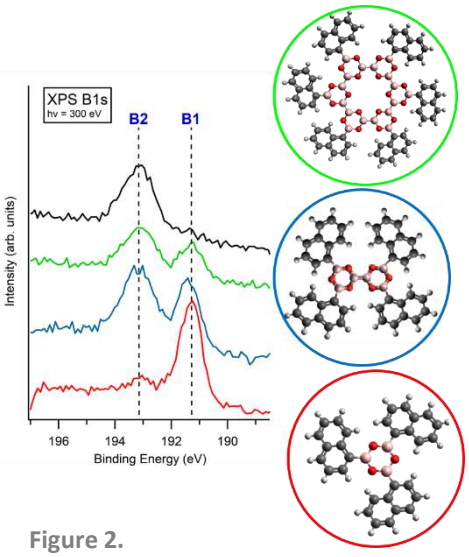

Figure 2.
B1s XPS taken in differently prepared systems, i.e. different sample temperature depositions.

Unveiling the quantum nature of plasmons in metallic nanoparticles with electron beams

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Advances in electron microscopy have enabled the study of metal nanoparticles with subnanometer spatial resolution, providing a powerful tool for characterizing plasmonic excitations [1]. Most theoretical works describe the nanoparticles as spherical objects, although electron energy loss spectroscopy (EELS) which is sensitive to the shape of the target, reveals the influence of atomic scale features and faceted boundaries in the loss spectra.

We performed calculations of the EEL probability in isolated icosahedral clusters composed of 380 Na atoms using both and an efficient atomistic ab-initio TDDFT code [2], and a continuous classical BEM [3] method within a local dielectric framework. Three different shapes were considered for the latter (radius~2 nm),): a sphere, a regular icosahedron, and a smoothed irregular icosahedron resembling the electron density landscape obtained within atomistic TDDFT.

The results prove a high dependence of localized surface plasmons (LSPs) on the shape of the particles and the particular trajectory of the electrons and the failure of the classical description to address the spectral structure of confined bulk plasmons (CBPs). We use an additional spherical hydrodynamic model [4] to analyze the CBP excitations obtained in the TDDFT calculations. These findings bear out the importance of a proper consideration of the atomic-scale shape of nanoparticles in EEL spectroscopy, while highlighting the strengths and limitations of classical approximations to nanophotonics.

References

[1] A. L. Koh, K. Bao, I. Khan, W. E. Smith, G. Kothleitner, P. Nordlander, S. A. Maier, D. W. McComb, ACS Nano, 3, 3015-3022 (2009); S. Kadkhodazadeh, J. Rosenkrantz de Lasson, M. Beleggia, H. Kneipp, J. Birkedal Wagner, K. Kneipp, J. Phys. Chem. C, 118, 5478– 5485 (2014).

[2] M. Barbry, P. Koval, F. Marchesin, R. Esteban, A. G. Borisov, J. Aizpurua, D. Sánchez-Portal, Nano Lett., 15, 3410-3419 (2015); M. Urbieta, M. Barbry, Y. Zhang, P. Koval, D. Sánchez-Portal, N. Zabala, and J. Aizpurua, ACS Nano, 12, 585–595 (2018).

[3] F. J. García de Abajo, A. Howie, Phys. Rev. B, 65, 115418 (2002); U. Hohenester, Comput. Phys. Commun, 185, 1177-1187 (2014).

[4] T. Christensen, W. Yan, S. Raza, A. P. Jauho, N. A. Mortensen, and M. Wubs. ACS Nano, 8, 1745–1758 (2014).

Figures

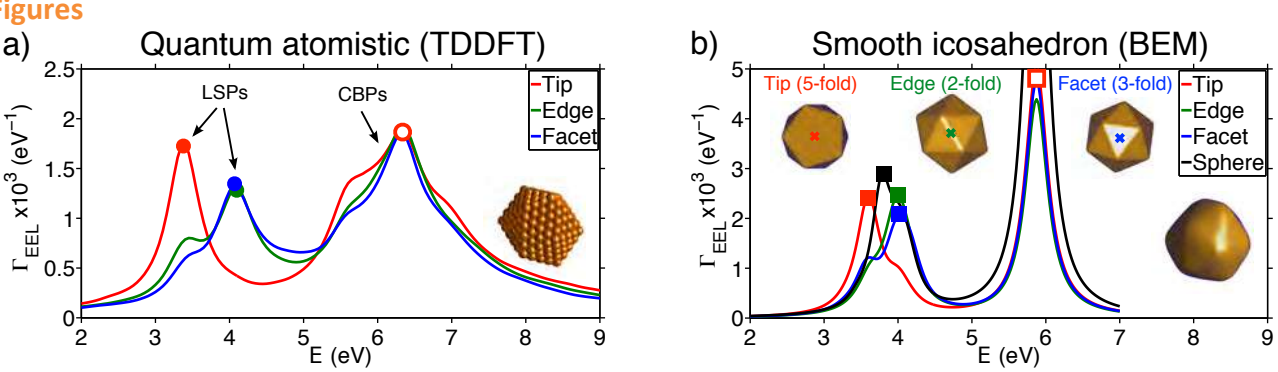

Figure 1. EEL spectra calculated for a) a Na380 cluster with TDDFT and b) an smoothed irregular icosahedron with BEM.

Preclinical safety of topically administered nanostructure lipid carriers (NLC) for wound healing application: biodistribution and toxicity studies

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Re-activation of the healing process is a major challenge in the field of chronic wound treatment. For that purpose, lipid-nanoparticles, especially nanostructured lipid carriers (NLC), possess extremely useful characteristics such as biodegradability, biocompatibility and long-term stability, besides being suitable for drug delivery [1]. Moreover, they maintain wound moisture due to their occlusive properties, which have been associated with increased healing rates. In the light of above, NLC have been extensively used topically for wound healing; but to date, there are no safety-preclinical studies concerning such type of application. Thus, in this work, biodistribution studies were performed in rats with the NLC previously developed by our research group, using technetium-99m (^{99m}Tc-NLC) as radiomarker, topically administered on a wound. ^{99m}Tc-NLC remained on the wound for 24 h and systemic absorption was not observed after administration (Figure 1). In addition, toxicological studies were performed to assess NLC safety after topical administration. The results obtained demonstrated that NLC were non-cytotoxic, non-sensitizing and non-irritant/corrosive. Overall, it might be concluded that developed NLC remained at the administration area, potentially exerting a local effect, and were safe after topical administration on wounds.

References

[1] Naderi N, Karponis D, Mosahebi A, Seifalian AM. Nanoparticles in wound healing; from hope to promise, from promise to routine. Frontiers in bioscience (Landmark edition) JID – 101612996

Figures

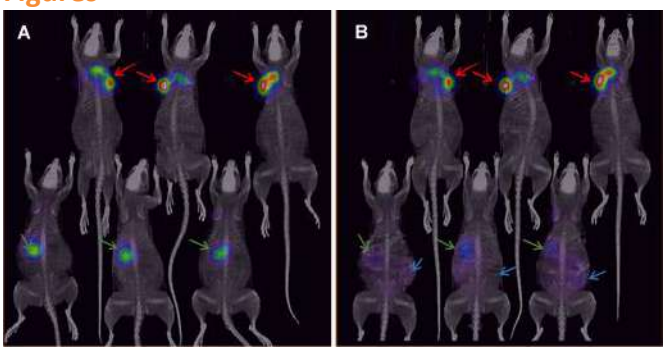

Figure 1. 3D images of the SPECT/ CT studies at 1 hour (A) and 24 hours (B). The three rats in the upper part of the image were treated with ^{99m}Tc-NLC on the wound area (red arrow), producing a stable signal over time. The three rats at the bottom of the image were control animals receiving free ^{99m}Tc on the wound. The green arrows indicate the stomach area, more evident at early times, and the blue arrows point to the large intestine.

Spatiotemporal mapping of heat and charge transport in $MoSe_2$

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The advent of 2D materials into the scientific (and technological) arena has been an interesting development during the last decade. Understanding nanoscale heat transport phenomena in these materials is of great importance, as it has an impact on the fields of photonics, thermoelectrics, and photodetection. Nevertheless, the phonon transport in these 2D materials is not explored to the same extent that their electrical and optical properties have been. Here we use the method of mechanical exfoliation to get large, atomically thin layers of $MoSe_2$, which are suspended over holes large than 10 microns. For exfoliation, we use PDMS stamps and blow with a nitrogen gun for better contact between the substrate and the non-suspended part of the flake. It is necessary to prepare free-standing, suspended $MoSe_2$ flakes, in order to avoid out-of-plane heat sinking into a supporting substrate. In large (>10 microns) suspended flakes, we often observe wrinkles at the time of transferring or after storing the sample in ambient conditions. We found that these wrinkles can be removed by a heating cycle (150 ºC for 30 min).

These suspended $MoSe_2$ samples are investigated using optical methods to study their intrinsic thermal properties. Two complementary optical techniques: Raman thermometry [1] and ultrafast spatiotemporal mapping [2], are used in our experiment. These two techniques probe different heat transport parameters – thermal conductivity (κ) and diffusivity (D) respectively – and therefore both separately, and together they provide information regarding the heat transport in the system. Raman thermometry uses a CW laser to assess the temperature-dependent Raman shift of the A_{1g} peak, and then the information on thermal conductivity is extracted by fitting the temperature profile. Using ultrafast spatiotemporal mapping, we combine spatial (~20 nm) and temporal (~200 fs) resolution for the study of heat carrier dynamics. Here we vary both time delay as well as spatial displacement between two femtosecond laser pulses to obtain the diffusivity of the sample. Our preliminary data show an agreement between the obtained transport parameters and with literature [3]. We further discuss our ongoing efforts on determining the different parameters that can affect thermal conductivity and diffusivity of suspended $MoSe_2$ crystals of varying thickness.

References

[1] Sledzinska, M., Graczykowski, B., Placidi, M., Saleta Reig, D., El Sachat, A., Reparaz, J. S., Alzina, F., Mortazavi, B., Quey, R., Colombo L., Roche, S., and Sotomayor Torres, C. M., *2D Materials,* vol. 3, p. 035016, (2016).

[2] Block, A., Liebel, M., Yu, R., Spector, M., Sivan, Y., García de Abajo, J. F., and van Hulst, N. F.,*Science Advances,* vol. 5, eaav8965, (2019).

[3] Morell, N., Tepsic, S., Reserbat-Plantey, A., Cepellotti, A., Manca, M., Epstein, I., Isacsson, A., Marie, X., Mauri, F. and Bachtold, A., *Nano letters*, *19*(5), pp.3143-3150, (2019).

Tuning the electronic and magnetic properties of β_{12}-borophene

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In last years, enormous research has been focused on two-dimensional (2D) nanomaterials due to their attractive physical properties and various technological applications. Recently, two-dimensional (2D) boron sheets named as borophene have been synthesized on silver surfaces [1-2]. Borophene exhibits various structural polymorphs, all of them metallic and highly anisotropic. However, pristine borophene is inherently non-magnetic, which limits its use for spintronic applications. Several approaches can be used to induce magnetic properties in borophene. For example, the adsorption of 3d transition metals (TM) or the patterning of borophene into 1D strips, named as borophene nanoribbons (BNRs) [3-4].

In this work, by using density functional theory (DFT), we investigate the changes in the electronic and magnetic properties of one of the polymorphs of borophene, called β_{12}, when TMs are adsorbed on it. Our calculations show that the electronic structure and the magnetic properties of borophene can be tuned by 3d TM atom adsorption, as shown in Figure 1. Based on the results for TM adsorption on extended β_{12}, the electronic transport properties of pristine and TM-doped β_{12}-BNRs will be explored. Our findings will be useful for the design of future borophene based spintronic devices.

References

[1] Mannix, A. J. *et al*. Science 350, 1513 (2015).
[2] Wang, H. F. *et al*. New J. Phys. 18, 073016 (2016).
[3] Sevinçli, H. *et al.* Phys. Rev. B 77 195434 (2008).
[4] Sahar Izadi .S. *et al.* Nanomicro Lett. 10 (2018).

Figures

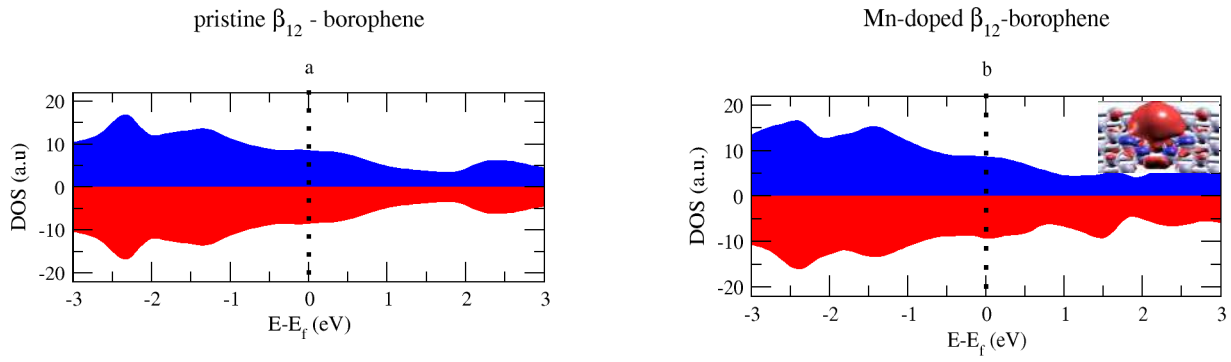

Figure 1. Density of states (DOS) of (a) pristine and (b) Mn doped borophene. The inset in (b) shows the spin density ($\rho\uparrow-\rho\downarrow$) isosurface distribution (0.0005eV/Å^3)

Magnetic order and electronic structure of lanthanide-containing thallium dichalcogenides

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One of the most promising approaches for realizing the quantum anomalous Hall effect is the magnetic extension of topological insulator [1]. To date, a number of promising systems have been proposed, based on topological insulator (TI) and magnetic thin films. The magnetic insulator in such a system has to satisfy a number of conditions. It has to have the same crystal structure as the TI, while its lattice parameter and work function should be close to those of the TI. In such a case, the heterostructure is guaranteed against appearance of harmful trivial interfacial states that could make the system spectrum gapless.

The thallium-based TIs $TlAX_2$ (*A* = Sb, Bi, *X* = Se, Te) family has been discovered in 2011. However, a suitable isostructural magnetic insulator to form a magnetic extension has not been reported so far. In this work, by means of *ab initio* calculations we have studied magnetic and electronic structure of lanthanide-containing thallium dichalcogenides $TlLnX_2$ (*Ln* = Gd, Eu, *X* = Se, Te) in order to check whether these materials are suitable to be a magnetic extension of the thallium-based TIs. Our results indicate that the intralayer FM ordering is favorable for $TlEuTe_2$, while for other three compounds a noncollinear antiferromagnetic 120° structure has the lowest energy. The gadolinium-based compounds were found to be semiconductors, while the europium compounds are metals, which, however, show a band gap in the conduction band.

Although the semiconducting systems studied here do not show desirable ferromagnetic order, the weak intralayer magnetic coupling theoretically makes it possible to control magnetic order by means of the external magnetic field. For example, the quantized Hall effect [2-3] has been measured in the $MnBi_2Te_4$ antiferromagnet that has been drive in the ferromagnetic state by the external magnetic field.

This work was funded by Russian Foundation for Basic Research within the research project № 18-32-00728.

References

[1] Otrokov M. M. *et al.* 2D Materials 4(2), 025082 (2017).
[2] Y. Deng, et al., arXiv:1904.11468 (2019).
[3] C. Liu, et al., arXiv:1905.00715 (2019).

Optical and electrical characterization of CuO/ZnO heterojunctions

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The lack of p-type electrical conductivity in ZnO emphasizes the importance of the study of hybrid heterojunctions. Among different p-type materials, copper oxide is a good candidate to create a p-n heterojunction with ZnO with a broad application potential in different optoelectronic devices. The main advantage of copper oxide is nontoxicity, low market price, and high absorption coefficient. The combination of p-type copper oxide and n-type zinc oxide appears promising for the implementation in photovoltaic devices with copper oxide as an absorbing layer and wide band gap zinc oxide as a windows layer. Another application area is gas sensing; however, metal oxide sensors suffer from poor selectivity. The selectivity can be enhanced by the fabrication of p-n junctions between different metal oxides.

In this work we present a cost-effective technology for the preparation of coper oxide/zinc oxide heterojunctions. The p-n heterojunctions were fabricated by sputtering of a metallic Cu thin film on top of solution grown ZnO nanorod arrays followed by thermal annealing at 400°C. Structural, morphological, and optical properties of both copper thin films and zinc oxide nanorod arrays were studied. The electrical properties of the junction were investigated by current-voltage and impedance spectroscopy measurements. Electrical characteristics of these junctions are sensitive to gas mixtures with a low hydrogen concentration and show fast response and recovery time. The copper oxide/zinc oxide heterojunction is shown to be more efficient to hydrogen detection at room temperature in comparison with the resistivity sensor based on zinc or coper oxides.

This work was supported by the Czech Science Foundation project 19-02804S.

Figures

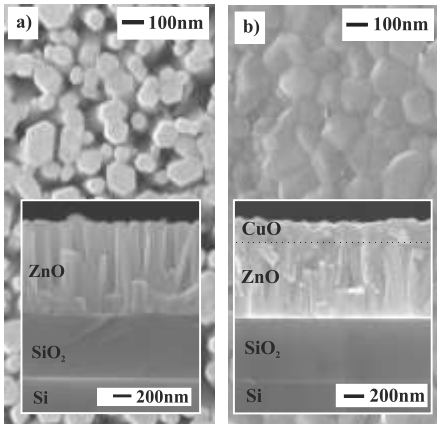

Figure 1. Top-view and cross-sectional SEM images of (a) ZnO nanorods; (b) copper oxide/zinc oxide heterojunction.

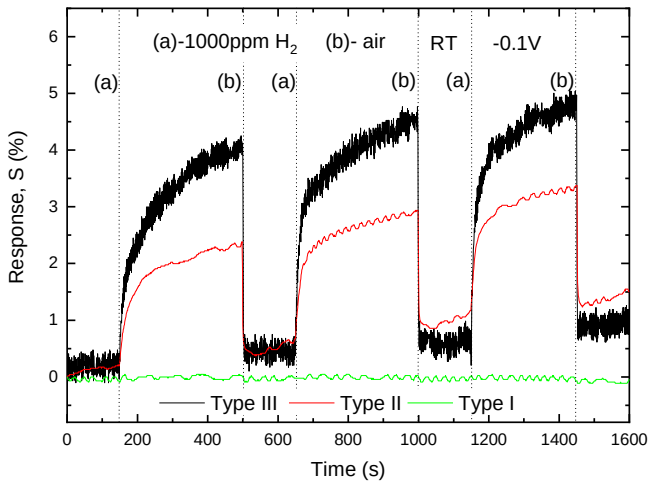

Figure 2. The room temperature transient response measured at -0.1 V. Type I - resistivity sensor based on copper oxide; Type II - resistivity sensor based on zinc oxide nanorods; Type III - copper oxide/zinc oxide p-n heterojunction sensor.

Reduction of non-specific interactions in systems based on PAMAM dendrimers for targeted MRI contrast agent delivery

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Introduction

Non-invasive specific diagnosis of tumor diseases can be achieved by using imaging technics like MRI with contrast agents. Low-molecular contrast agents, suffer from rapid elimination from blood vessels, leading to a rapid decrease in the concentration of the substance. In this regard, it is required to apply higher concentrations of contrast agents, which increases the cost and toxicity of the procedure [1]. For this purpose, it is more suitable to use high-molecular contrast agents, like polyamidoamine (PAMAM) dendrimers with conjugated chelated forms of Gd(III) on its surface. The use of dendrimers which have a lot of terminal surface groups makes it possible to conjugate a large number of chelate groups on the surface, increasing the local concentration of the contrast agent, which greatly increases the relaxation and effectiveness of contrast agent [2]. For more selective tumor contrast, vector molecules which are directed at overexpressed tumor markers on the surface of cancer cells, such as alpha-fetoprotein (AFP) [3], may be used.

Materials and Methods

PAMAM-DOTA conjugate were synthesized using PAMAM-NH2 dendrimers (generations G2 and G3) and DOTA-NHS ester. Conjugation of vector molecule (third domain of AFP (3DAFP)) were done through carbodiimide intermediate. Size and zeta-potential of both products (DOTA-PAMAM G2.0 and DOTA-PAMAM G3.0) were characterized by dynamic light scattering (DLS) and electrophoresis. The number DOTA groups conjugated onto each dendrimer surface were determined by ^{1}H NRM and MALDI-TOF. After chelation the amount of gadolinium were determined by atomic-emission spectroscopy. Specific and non-specific interaction between cells and dendrimers were tested in vitro on MCF-7 and SCOV-3 cell lines.

Results

Synthesized DOTA-PAMAM G2.0 and DOTA-PAMAM G3.0 had an average diameter of 6 to 18 nm and zeta potential in range from +33.8±5.12 mV to -21.8±2,48. The results of 1H NRM shows expected level of DOTA to dendrimer surface and atomic emission spectroscopy data reveals chelation of Gd(III) ions by all DOTA groups. The results of non-specific interactions between PAMAM-DOTA-Gd(III) showed increase of dendrimer binding to cell surface with high positive surface charge, negatively charged macromolecules showed reduced binding. At the same time, negatively charged dendrimers conjugated with 3DAFP showed increased specific binding and accumulation in MCF-7 and SCOV-3 cell lines.

Conclusion

Non-specific interactions of PAMAM-DOTA-Gd(III) greatly depends from zeta potential of macromolecule. Dendrimers with more positive zeta potential binds to the cells non-specifically due to negative charge of cell walls. Negatively charged dendrimers interact with cells less but with addition of vector molecule specifically binds to tumor cells without non-specific binding. This work was supported by the grant of Russian Foundation for Basic Research (No. 18-29- 09022\18).

References

[1] Aime S. et al. Magn. Reson. Imaging., 2009., 30 (6)., 1259-1267
[2] Aaron J. et al. Chem. Rev., 2010., 110 (5)., 2921-2959
[3] Ricardo M. Alpha-Fetoprotein: Functions and Clinical Applications., 2016, Ch. 14., 241-275

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