Identification of Twisted Bilayer Transition Metal Dichalcogenides by Combination of Deep learning and OpenCV

Yong Xie[1,2]*, Haitao Yang[2], Kexin He[2], Daniel Yélamos[1], Eduardo Robert Rafael Hernández [1], Andres Castellanos-Gomez [1]

[1]*Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, 28049 Madrid, Spain.*

[2]*School of Advanced Materials and Nanotechnology, Xidian Univ., Xi'an 710071, China*

xieyong.nwpu@gmail.com

Two-dimensional materials are expected to play an important role for the next generation electronics and optoelectronic devices. Up to date, the high quality two-dimensional are made by either mechanical exfoliation or chemical vapor deposition (CVD). In addition, twisted bilayer graphene or transition metal dichalcogenides (TMDs) gain more attention for their rich physics and applications. In this paper, based on the color space of chemical vapor deposition (CVD) molybdenum disulfide (MoS_2) collected by optical microscopy (OM), the semantic segmentation convolutional neural network (CNN) is used to achieve accurate recognition and rapid identification of MoS_2 by using different models. Moreover, the image processing algorithm using OpenCV is implemented to further characterize the twisted angles features of materials. Our results pave the way for the automatic inspection of twisted TMDs in large scale.

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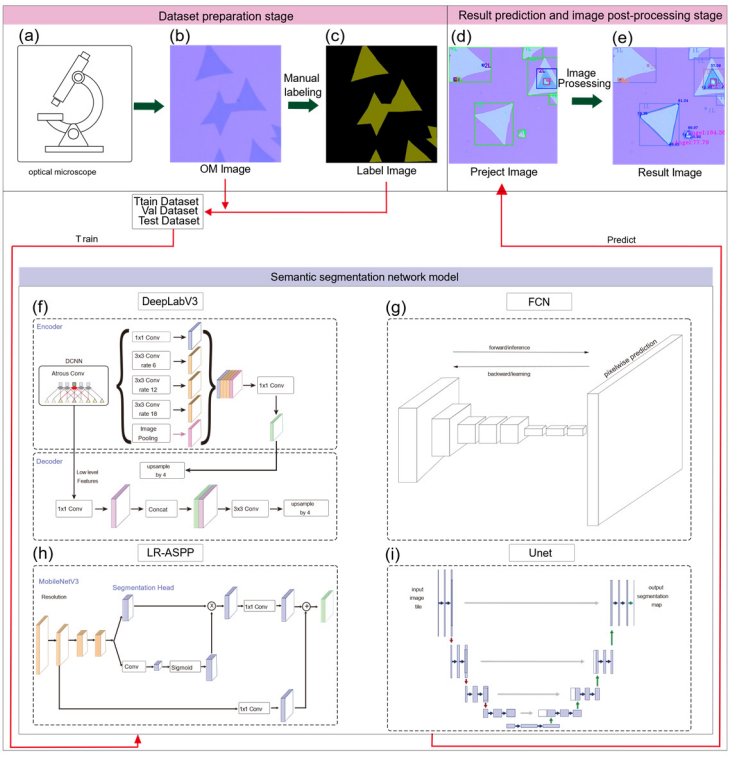

Figure 1: The process of identification of twisted bilayer TMDs.

Energy tunable of Single Photon Emitters in Hexagonal Boron Nitride by Ion Irradiation

Abel Martínez-Suárez[1,2]
Adam Roselló[1,3], Dimas Oteyza[2,3], Aitana Tarazaga Martín-Luengo[1], Stefan Partel [4], Sandra Stroj [4], Pablo Alonso-González[1,2], Javier Martín-Sánchez[1,2]
[1]*Departamento de Física, Universidad de Oviedo, Oviedo, Spain*
[2]*Nanomaterials and Nanotechnology Research Center (CINN-CSIC), El Entrego, Spain*
[3]*Donostia International Physics Center (DIPC), Donostia/San Sebastián, Spain*
[4]*Research Center for Microtechnology Vorarlberg University of Applied Sciences Hochschulstraße Dornbirn , Austria*
martinezabel@uniovi.es

The development of novel ultra-compact two-dimensional (2D) photonic technologies for application in quantum information processing, relies on our ability to fabricate single photon sources in 2D van der Waals materials with control of their optical emission properties, and preferably working at room temperature (RT). Recently, the possibility of obtaining single photon emission from 2D hexagonal boron nitride (h-BN) crystals at RT has been demonstrated, attributed to the presence of defects states within its wide bandgap [1], which has triggered an intense research activity in the last years [2]. In this regard, the deterministic fabrication of such emitters in h-BN has been tackled by different techniques such as thermal annealing [3], plasma treatment [4] or electron irradiation [5].

In this work, we present a novel approach to the deterministic induction of strain induced single photon emitters with energy control by using piezoelectric columns. Specifically, a set of samples consisting of thin 2D h-BN flakes obtained by mechanical exfoliation has been iradiated on triangular columns and pillars. We clearly observe a shift on the emission from the pillars where quantum emitters are induced flakes in comparison with pristine flakes where a relatively low density of emitters is measured. The emission energy in irradiated h-BN 2D crystals is discussed based on micro-photoluminescence, time-resolved, time-correlated characterizations and strain measurements.

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Strong exciton-phonon coupling in semiconducting monolayer *2H*-$MoTe_2$

Jorge Cervantes Villanueva[3]
Charles J. Sayers[1], Alberto García-Cristóbal[3], Armando Genco[1], Chiara Trovatello[1], Stefano Dal Conte[1], Vladislav Khaustov[2,5], Camilla Coletti[2,6], Christoph Gadermaier[1], Giulio Cerullo[1], Davide Sangalli[4] and Alejandro Molina-Sánchez[3]
[1] *Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy*
[2] *Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, 56127 Pisa, Italy*
[3] *Institute of Materials Science (ICMUV), University of Valencia, Catedrático Beltrán 2, E-46980 Valencia, Spain*
[4] *Istituto di Struttura della Materia-CNR (ISM-CNR), Division of Ultrafast Processes in Materials (FLASHit), Area della Ricerca di Roma 1, Monterotondo Scalo, Italy*
[5] *Scuola Normale Superiore, piazza San Silvestro 12, 56127 Pisa, Italy*
[6] *Graphene Laboratories, Istituto Italinao di Tecnologia, 16163 Genova, Italy*
Jorge.cervantes@uv.es

The coupling of the electrons to lattice vibrations and their time-dependent control and detection provides unique insight into the non-equilibrium physics of semiconductors. *2H*-$MoTe_2$ is a transition metal dichalcogenide (TMD) that has not been extensively studied in this way due to its low chemical stability, which has recently solved by encapsulation using few-layer hBN **[1]**. Optical pump-core level (XUV) probe spectroscopy has revealed a strong oscillatory signal contribution dominated by the out-of-plane A_{1g} phonon mode **[2]**. In this work we perform a theoretical analysis of the non-equilibrium optical properties of *2H*-$MoTe_2$ by means of *ab-initio* simulations combining density functional (and perturbation) theory (DFT/DFPT) and many-body perturbation theory (GW+BSE). The calculations are performed with both equilibrium atomic positions and with the atoms displaced simulating the A_{1g} phonon mode, Fig (a). We find a rearrangement of the optical absorption of monolayer $MoTe_2$ in the region 1.7 – 2.2 eV, Fig (b), due to the strong exciton-phonon coupling of the B' exciton. Our results highlight the extreme sensitivity of the optical properties of monolayer TMDs to small structural modifications and their manipulation with light.

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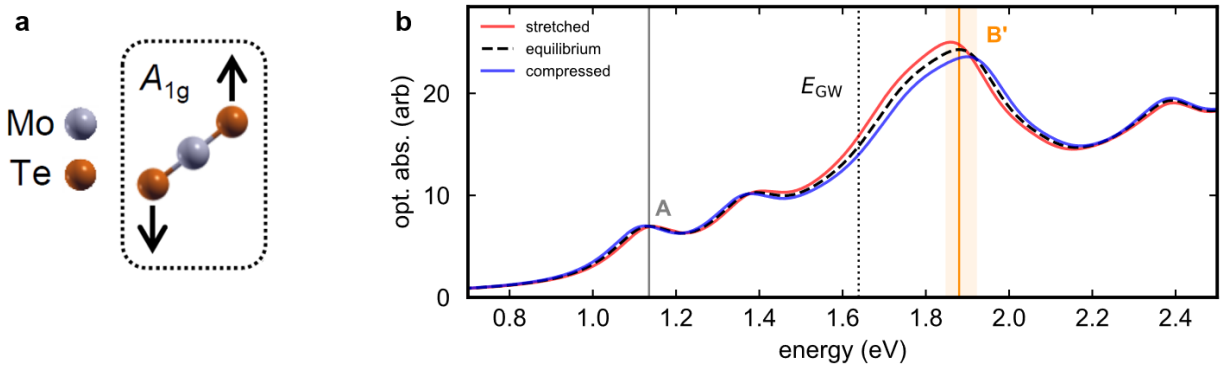
Figure



Electronic correlations in the normal state of twisted bilayer graphene

María José Calderón[1]
Anushree Datta[1,2], Alberto Camjayi[3], Elena Bascones[1,2]

1. *Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, Sor Juana Inés de la Cruz 3, 28049 Madrid (Spain)*
2. *Laboratoire Matériaux et Phénomènes Quantiques and Laboratoire de Physique des Solides, Paris (France)*
3. *Ciclo Básico Común, Universidad de Buenos Aires and IFIBA, Conicet, Pabellón 1, Ciudad Universitaria, 1428 CABA, Argentina*

mariaj.calderon@csic.es

The discovery of insulating states, superconductivity and other broken symmetry states in magic angle twisted bilayer graphene [1] and other graphene multilayers [2] has marked a new era in the research of correlated materials. In these systems, narrow bands can lead to an enhanced importance of interactions on the electronic properties both in symmetry broken and in non-ordered states. We will focus on the case of twisted bilayer graphene and will show the effect of correlations in its normal, non-ordered state, using dynamical mean field theory on an 8-orbital model [3] including all important, both short and long range, interactions [4]. Correlations lead to a strong reorganization of the spectral weight that can have important consequences for the electronic properties of both the normal and the ordered states.

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Twisted devices from CVD graphene

Sergio Pezzini
NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza San Silvestro 12, Pisa 56127, Italy
sergio.pezzini@nano.cnr.it

Twisted 2D materials provide an extraordinarily rich platform for engineering emergent electronic, magnetic, and optical properties. However, to help realizing the applicative potential of *twistronics*, synthesis and assembly techniques need to meet stringent requirements in terms of device-scale interface cleanness and twist-angle control.
We present recent advancements in the realization of dual-gated high-mobility devices based on twisted graphene layers synthesized via chemical vapor deposition (CVD). On the one hand, large-angle twisting can be stabilized at the growth stage [1], ensuring electronic decoupling and parallel transport between pristine graphene sheets with a gate-controlled carrier distribution [2]. On the other hand, small-angle configurations can be selected via hBN-mediated stacking of two separated crystals grown on a single Cu grain [3]. Low-temperature magnetotransport is employed to reveal the hallmarks of a 2.4°-twisted superlattice, including tunable regimes of interlayer coupling, reduced Fermi velocity, large interlayer capacitance, and density-independent Brown-Zak oscillations (see Figure 1).

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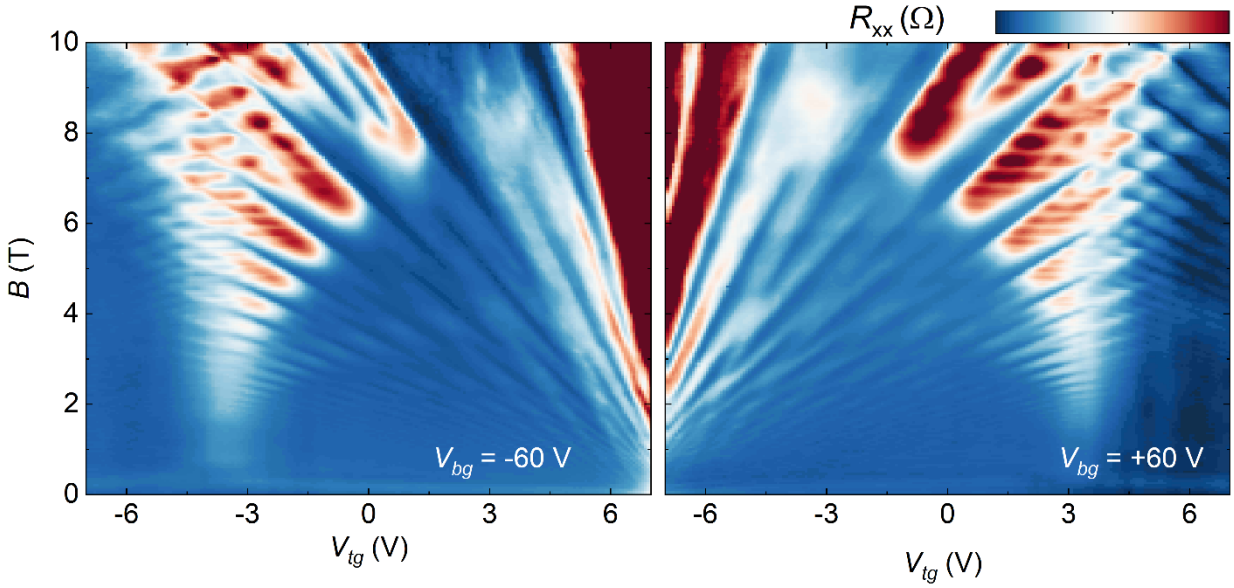

Figure 1: Longitudinal resistance of 2.4°-twisted bilayer graphene as a function of the top-gate voltage (at two different back-gate values), and the magnetic field. Oppositely-dispersing Landau fans coalesce at low-energy van Hove singularities (light red funneling regions). Density-independent Brown-Zak oscillations (horizontal features) arise due to commensurability of the magnetic length and the superlattice periodicity. Adapted from Ref. [3].

High harmonic generation with a twist: all-optical characterization of magic-angle twisted bilayer graphene.

Eduardo B. Molinero
A. Datta, E. Bacones, M. J. Calderón, R. E. F. Silva.
Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Sor Juana Inés de la Cruz 3, 28049 Madrid (Spain).
e.b.molinero@csic.es

The discovery of magic-angle twisted bilayer graphene [1] has led to the birth of a promising new field of condensed matter physics based on moiré quantum materials. In parallel, the study of ultrafast electronic dynamics in condensed matter systems has also experienced a huge growth in relevance [2]. In the present work, we aim to bridge the gap between these two distinct fields by studying high-harmonic generation in magic-angle twisted bilayer graphene. Indeed, we will show that one can characterize the magic angle in a fully optical way.
When we twist the two grapene layers close to the magic angle, a decrease of several orders of magnitude in the harmonic intensity can be appreciated, see Fig. 1. This decrease is crucially related to the appereance of a pair of flat bands at that specific angle. Additionally, we show that, despite the complexity of the system, the physical picture can be understood quite easily thanks to the use of a semiclassical model.
Surprisingly, this effect is shown to be robust under variations of the laser field, showing no anisotropy in the laser direction. Furthermore, it does survives up until cryogenic temperatures, far away from the usual experimental range of temperatures. We hope that our work can shed light onto the mechanisms behind electronic ultrafast dynamics in twisted materials.

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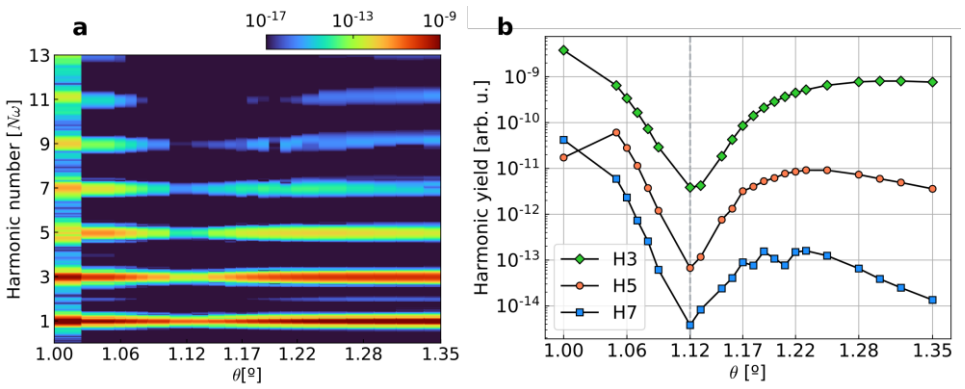

Figure 1: a, harmonic intensity in terms of the twist angles and the harmonic number. **b**, harmonic yield for the third, fifth and seventh harmonics in terms of the twist angles.

Memristive behaviour in exfoliated and nanostructured three-terminal MoS_2 devices
(Times New Roman 15)

G. Caballero[1]
J. Garcia[1], F. J. Urbanos[1], F. Aguirre[2], R. Bernardo-Gavito[1], E. Miranda[2], M. Menghini[1] and D. Granados[1]
[1]IMDEA Nanociencia, 28049 Madrid, Spain
[2]Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona (UAB), 08193 Barcelona, Spain
Email: gabriel.caballero@imdea.org

Two-dimensional materials possess great potential as core active materials for novel electronic, optoelectronic and sensing applications. In particular, transition metal dichalcogenides (TMDs) and other low-dimensional materials, such as hexagonal Boron Nitride (hBN), have exhibited memristive behaviour [1]. This makes them attractive candidates as building blocks for resistive memories and neuromorphic computing devices [2].

This work presents three-terminal field-effect transistor devices (memtransistors [3]) based on mechanically exfoliated MoS_2 flakes. We used a Gas Injection System (GIS) to modify the device geometry using xenon difluoride as the etchant gas. In general, the devices suffer a doping change due to the formation of sulphur vacancies during the etching process [4], which gives rise to interesting IV characteristics not present in the pristine devices. We have studied the electrical properties and memristive-like behaviour in freshly exfoliated and nanostructured devices both in air and in vacuum, as well as a function of the temperature in the 300K to 77K range. We observed a progressive amplification of the device conductance, followed by a partial reset for positive voltage sweeps. The devices present wipe-out properties under negative bias. We have performed simulations of the device conductance using the dynamic memdiode model [5] that reasonably reproduces the experimental results.

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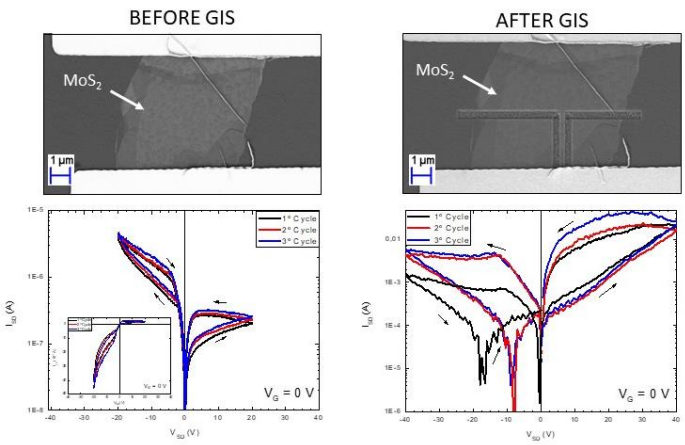

Figure 1: Characteristic curves before and after nanopatterning process.

Performing an array of MoS_2 micro-drum resonators

Julia García-Pérez[1], Víctor Marzoa[1], Ramón Bernardo-Gavito[1] and Daniel Granados[1]
[1] *IMDEA Nanociencia, Calle Faraday 9, Madrid, Spain*
julia.garcia@imdea.org

Nanoelectromechanical systems (NEMS) is a sort of device capable of transducing an electrical signal to a mechanical motion or the other way round. In particular, drum resonators based on two-dimensional materials have been thoroughly studied in the last few years due to their mechanical properties and potential applications, such as sensors [1]. This work studies the electrical and optical properties of micro-drum resonators fabricated with mechanically exfoliated few-layer MoS_2.

By applying DC and RF electric fields between the top electrode and the bottom of the covered well (Si [N++]), we induce mechanical oscillations in the suspended region, studying the resonant membrane's motion at the nanoscale. Readout of the mechanical movement of the membrane is performed via changes in the system's reflectivity.

Changing the number of layers will modify the pre-tension and the effective mass of the membrane of the drum thus it will vary the resonance frequency of the system [2]. We study the electro-mechanical response of an array of five micro-drum resonators both at atmospheric pressure and in high-vacuum, in this last case, at room temperature and cryogenic conditions. We observe the evolution of the fundamental mode, the first vibrational harmonic and their transition from the linear to the non-linear regime under different excitation conditions to each micro-drum.

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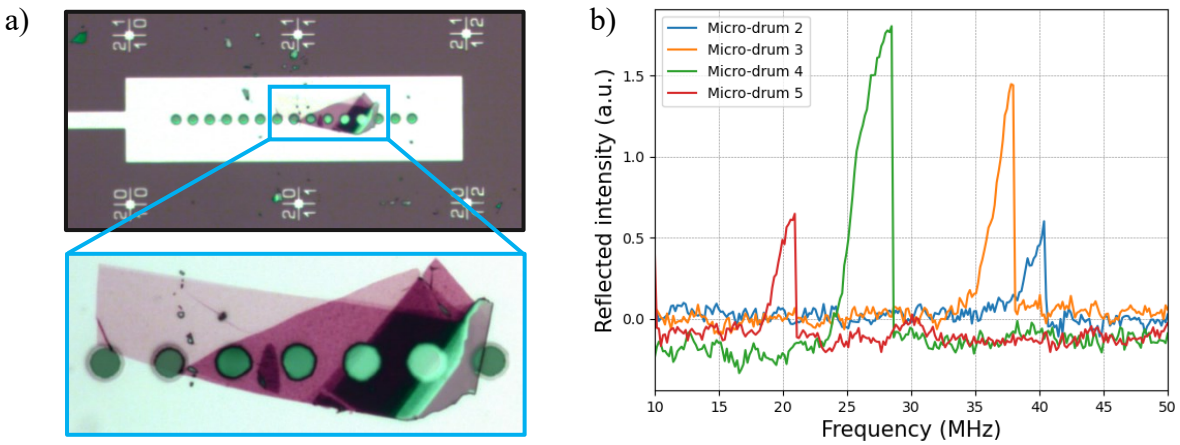

Figure 1: a) Micrograph of the system. MoS_2 flake with different number of layers onto five well-defined wells. b) Resonance frequency of four micro-drum.

Highly tunable opto-electrical response in $FePS_3$-MoS_2 van der Waals p-n heterojunctions

Marcos Gadea[1], María Ramos[1], Samuel Mañas[2], Eudomar Henríquez[1], Eugenio Coronado[2], M. Reyes Calvo[1]*

[1]*Departamento de Física Aplicada and Instituto Universitario de Materiales de Alicante (IUMA), Universidad de Alicante, Campus de San Vicente del Raspeig, E-03690 Alicante, Spain*
[2]*Instituto de Ciencia Molecular (ICMol), Universitat de Valencia, Paterna 46980, Spain*

E-mail: marcos.gadea@ua.es

The unique properties of van der Waals semiconductor heterostructures provide versatility and added functionality to the design of optoelectronic devices. Here, we present p-n junction heterostructures built from n-type, single-layer MoS_2 and p-type, multilayer $FePS_3$, where electrical photo-response and robust photoluminescent light emission coexist. Firstly, we find that these heterostructures constitute p-n junctions suitable as broad-range photodiodes with best performance for ultraviolet photodetection. Our results show that the photo-response of the $FePS_3/MoS_2$ device is strongly sensitive to the application of an external electric field, which enables the precise tuning of the diode characteristics and the photodiode operation under reverse and forward bias. More interestingly, we explore the competition between photoluminescence and photocurrent generation and demonstrate that, in this system, light emission from single-layer MoS_2 can be controlled – from severely quenched to two orders of magnitude enhancement – by small changes in the applied bias voltage across the junction.

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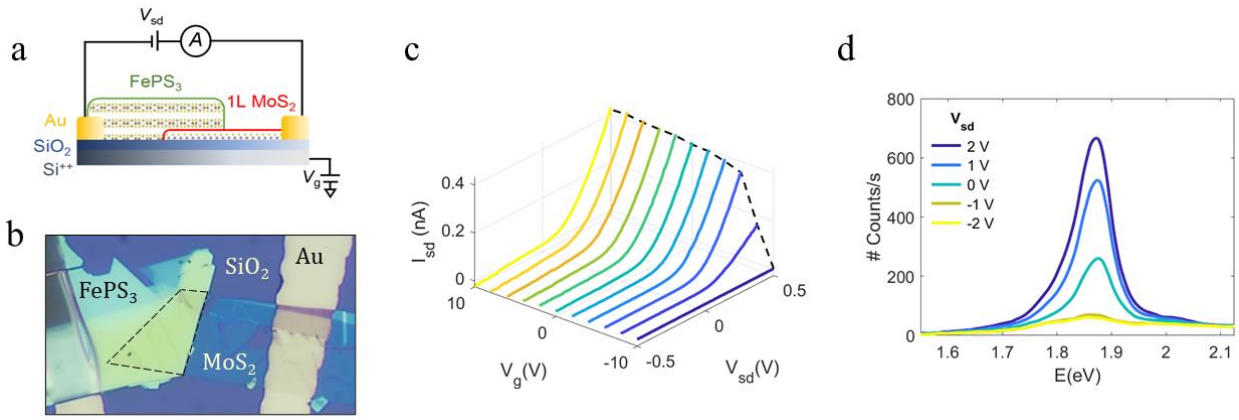

Figure 1: (a) Sketch for a device containing a multilayer $FePS_3$/ single-layer MoS_2 heterostructure. (b) Optical microscopy image of a heterostructure device (c) Source-drain current-voltage characteristics as a function of the applied back-gate voltage. (d) Photoluminescence emission of single-layer MoS_2 composing the $FePS_3$-MoS_2 heterojunction as a function of the applied bias voltage.

Study of the hydrodynamic electron flow regime in ultrapure 2D materials

Carlos Sánchez Sánchez, Juan Salvador, Ana Pérez-Rodríguez, Vito Clericò, Enrique Diez y Mario Amado.
Nanotechnology Group, University of Salamanca, Salamanca, Spain
carlos.sanchez@usal.es

The behavior of electron flow in metals at low temperatures sometimes deviates from the typical ohmic model found at normal temperature and pressure. At these low temperatures, electron-electron interactions can dominate over the dissipative ones associated with the ohmic regime and give rise to interesting new electronic properties where a hydrodynamic theory is required to describe their properties.

This electronic regime has been predicted for more than 50 years. However, only recently have sufficiently clean electron systems with a transport dominated by e-e collisions become available, showing a behavior characteristic of highly viscous fluids.

One of the materials suitable for the observation of this behavior is graphene, which due to its high purity and weak electron-phonon coupling makes it possible to analyze the hydrodynamic regime over a wide range of temperatures. Due to the low electrical resistance found in this regime, an application for new types of electronic devices could be possible in the future.

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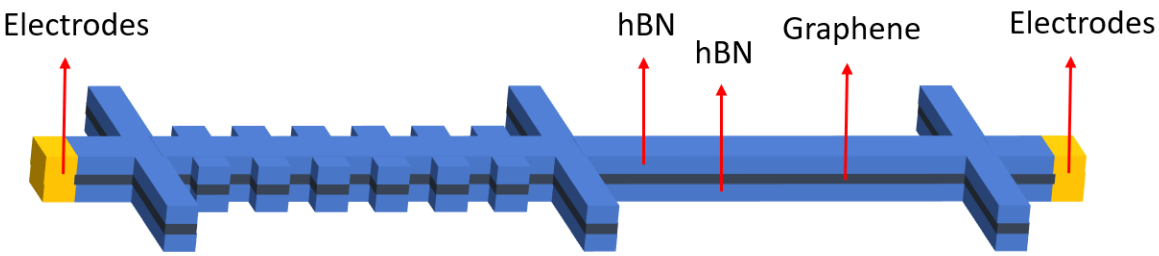

Figure 1: Image of the hBN-Graphene-hBN heterostructure device. The gate-defined channel contains two sections: a 2.5-µm-wide and 25-µm-long straight channel and a crenellated channel of the same dimensions with crenellations of 1 µm. In the crenellated channel, electrical resistance in the hydrodynamic regime is different from that in the ohmic regime, while the straight channel always offers the same resistance. Thus, the device is useful to characterize the hydrodynamic electron flow.

Photo-thermoelectric effect in $MnBi_2Te_4$ devices revealed by scanning photocurrent microscopy

Eudomar Henríquez-Guerra,
M. Reyes Calvo
Departamento de Física Aplicada – Instituto Universitario de Materiales IUMA
Universidad de Alicante, San Vicente del Raspeig, Alicante, España
eudomar.henriquez@ua.es / reyes.calvo@ua.es

$MnBi_2Te_4$ is a narrow gap semiconductor that, at low temperatures, hosts antiferromagnetic ordering and Anomalous Quantum Hall edge states. Furthermore, non-linear photocurrent responses have been predicted for this material. In this work, we study the photo-response of devices formed by $MnBi_2Te_4$ flakes with ~100nm of thickness deposited over gold electrodes by scanning photocurrent microscopy. Scanning photocurrent maps (such as the one shown in Fig. 1) at 4K show maximum current when the laser spot (λ=532nm) is placed on the $MnBi_2Te_4$/Au interface and surrounding regions. This behavior is typically associated with the photothermoelectric effect, the sample is locally heated by the light, creating a local increase of charge carriers that results in a diffusion current. This effect has been reported by other authors in MoS_2 [1] and black phosphorus [2, 3] devices. The strength of photothermoelectric effects on $MnBi_2Te_4$, could make this an interesting material for the design of thermo-electric nanodevices and photo-thermal sensors.

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Figures

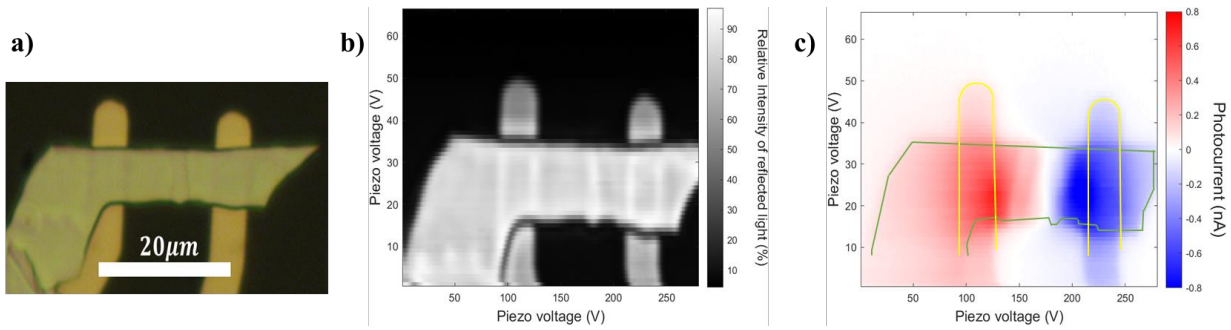

Figure 1: a) Optical microscopy image of a $MnBi_2Te_4$ device. b) Confocal microscopy map recorded simultaneously to c) Scanning photocurrent map for the device in a).

Negative reflection of nanoscale-confined polaritons in a low-loss natural medium

Enrique Terán García
Gonzalo Álvarez Pérez[1,2], J. Duan[1,2], J. Taboada-Gutiérrez[1,2], Q. Ou[3], E. Nikulina[4], S. Liu[5], J. H. Edgar[5], Q. Bao[3,6], V. Giannini[7,8,9], R. Hillenbrand[4, 10], J. Martín-Sánchez[1,2], A. Y. Nikitin[10,11], P. Alonso-González[1,2]
[1]*Department of Physics, University of Oviedo, Oviedo 33006, Spain.*
[2]*Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo), El Entrego 33940, Spain.*
[3]*Department of Materials Science and Engineering and ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET), Monash University, Clayton, Victoria, Australia.*
[4]*CIC nanoGUNE BRTA and Department of Electricity and Electronics, UPV/EHU, Donostia/San Sebastián 20018, Spain.*
[5]*Tim Taylor Department of Chemical Engineering, Kansas State University, Manhattan, KS 66506, USA.*
[6]*Nanjing kLight Laser Technology Co. Ltd., Nanjing 210032, China.*
[7]*Instituto de Estructura de la Materia (IEM), Consejo Superior de Investigaciones Científicas (CSIC), Serrano 121, Madrid 28006, Spain*
[8]*Technology Innovation Institute, Building B04C, Abu Dhabi P.O. Box 9639, United Arab Emirates*
[9]*Centre of Excellence ENSEMBLE3 sp. z o.o., Wolczynska 133, Warsaw, 01-919, Poland.*
[10]*IKERBASQUE, Basque Foundation for Science, Bilbao 48013, Spain.*
[11]*Donostia International Physics Center (DIPC), Donostia/San Sebastián 20018, Spain*
gonzaloalvarez@uniovi.es

Negative reflection occurs when light is reflected toward the same side of the normal to the boundary from which it is incident. This exotic optical phenomenon is not only yet to be visualized in real space but also remains unexplored, both at the nanoscale and in natural media. Here [1], we directly visualize nanoscale-confined polaritons negatively reflecting on subwavelength mirrors fabricated in a low-loss van der Waals crystal. Our near-field nanoimaging results unveil an unconventional and broad tunability of both the polaritonic wavelength and direction of propagation upon negative reflection. On the basis of these findings, we introduce a device in nano-optics: a hyperbolic nanoresonator, in which hyperbolic polaritons with different momenta reflect back to a common point source, enhancing the intensity. These results pave way to realize nanophotonics in low-loss natural media, providing an efficient route to control nanolight, a key for future on-chip optical nanotechnologies.

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Figures

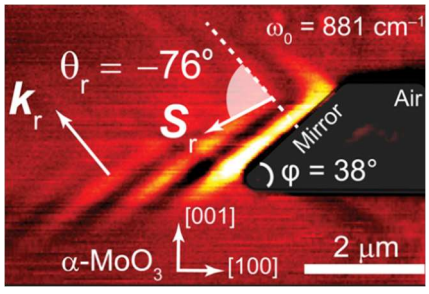

Figure 1: Visualization of negative reflection of nanoscale-confined polaritons in a natural medium.

Generation and control of non-local chiral currents in graphene superlattices by orbital Hall effect

Juan Salvador Sánchez[1]
1. Nanotechnolgy Group, Department of Fundamental Physics, University of Salamanca, 37008 Salamanca, Spain
juan2s@usal.es

Two-dimensional (2D) materials can be combined into complex heterostructures by stacking them with controlled twisted angles. Twisted layers of 2Ds present a modified band structure due to the presence of an induced Moiré pattern in their electronic structures [1]. This field of research, commonly known as *Twistronics*, has blossomed recently due to the discovery of exotic states of matter in twisted bilayer graphene devices [2].
Graphene-based superlattices offer a new materials playground to exploit and control a higher number of electronic degrees of freedom, such as charge, spin, or valley for disruptive technologies. Recently, orbital effects, emerging in multivalley band structure lacking inversion symmetry, have been discussed as possible mechanisms for developing orbitronics.
Here, we report non-local transport measurements in small gap hBN/graphene/hBN moiré superlattices which reveal very strong magnetic field-induced chiral response which is stable up to room temperature (Figure 1). The measured sign dependence of the non-local signal with respect to the magnetic field orientation clearly indicates the manifestation of emerging orbital magnetic moments [3]. The interpretation of experimental data is well supported by numerical simulations, and the reported phenomenon stands as a formidable way of insitu manipulation of the transverse flow of orbital information, that could enable the design of orbitronic devices.
There is no doubt that the study of different alignments among 2D materials opens many new possibilities in *Twistronics*, paving the way for new methods to obtain materials with novel quantum properties. In addition to their undoubted fundamental interest, these materials may also enable new quantum technologies that constitute a technological breakthrough.

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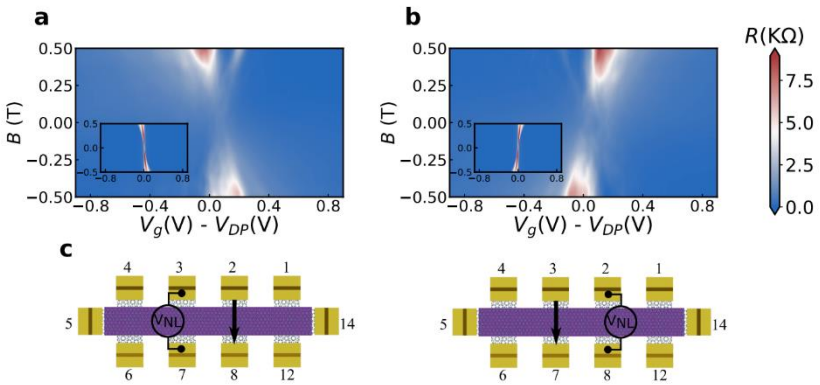

Figure 1: Panels and **a** and **b** show the heat maps of the sample non-local resistance for two symmetrical configurations scanned in the space of backgate voltage, corrected by the position of the Dirac peak at B = 0 (VG −VDP), and magnetic field measured at 250 mK. Insets on each graph show the numerical results for the OHE, showing extraordinary agreement with the experimental results. **c**, Sketch for the two different injection and collection configurations for the experimental and theoretical results shown in panels a and b above.

Nonlinear transport effects in chiral elemental Tellurium

Manuel Suárez Rodríguez[1]
F. Calavalle[1], B. Martín-García[1,2], A. Johansson[3,4], D. C. Vaz[1], H. Yang[1], I. Maznichenko[3], S. Ostanin[3], F. de Juan[2,5], S. Tsirkin[2,6], I. Sousa[2,6], A. Mateo-Alonso[2,7], A. Chuvilin[1,2], I. Mertig[3], M. Gobbi[1,2], F. Casanova[1,2], L. E. Hueso[1,2]
[1]*CIC nanoGUNE BRTA, 20018 Donostia-San Sebastian, Basque Country, Spain*
[2]*IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Basque Country, Spain*
[3]*Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle, Germany*
[4]*Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany*
[5]*Donostia International Physics Center, 20018 Donostia-San Sebastián, Basque Country, Spain*
[6]*Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain*
[7]*POLYMAT, University of the Basque Country UPV/EHU, 20018 Donostia-San Sebastian, Basque Country, Spain*
m.suarez@nanogune.eu

Chiral materials are an ideal playground for exploring the relation between symmetry, relativistic effects, and electronic transport [1]. Indeed, the role of low symmetry on electronic transport has been studied on chiral organic molecules, but their poor electronic conductivity limits their potential for applications. Conversely, chiral inorganic crystals, such as elemental Tellurium (Te), present excellent electrical conductivity and strong spin-orbit coupling [2]. Therefore, Te become a perfect material for studying the connection between nonlinear transport phenomena, such as unidirectional magnetoresistance (UMR) or nonlinear Hall effect (NLHE), and chirality [3]. Here, on one hand, we report a chirality-dependent and gate-tuneable Edelstein effect in naturally hole-doped Te nanowires (NWs) [4]. By recording a UMR dependent on the relative orientation of the electrical current and the external applied magnetic field, we link the direction of the spin polarization to the handedness of the crystal (Fig. 1). The measured UMR is explained on the basis of a chirality-dependent Edelstein effect arising from the radial spin texture at the H-point of the valence band of Te, which dominates the transport in our hole-doped Te NWs. In addition, an electrostatic gating enables the tuning of the Edelstein effect, leading to a modulation of the UMR amplitude by a factor of 6. On the other hand, we explore the NLHE in Te flakes. The symmetry of the measured second harmonic voltage under zero field, which is a consequence of the inversion symmetry breaking in Te, follows strictly the constrains for Te point group and is different from any material reported before. The all-electrical generation, control, and detection of spin polarization and second-order voltage in chiral Te NWs open the path to exploit chirality in the design of solid-state spintronic and energy harvesting devices.

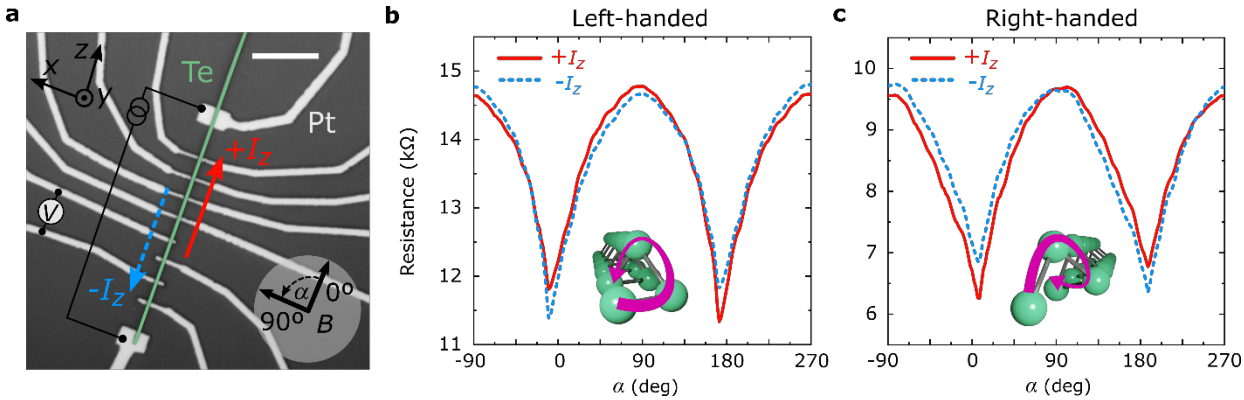

Figure 1: a, Te NW contacted with Pt contacts (the scale bar corresponds to 10 μm). **b**,**c**, Angular dependences of the magnetoresistance measured at 9 T and 10 K for two Te NWs with opposites handedness. Solid and dashed lines indicate the signal obtained from opposite current directions ($\pm I_z = \pm 1$ μA in **b** and $\pm I_z = \pm 0.7$ μA in **c**).

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Negative reflection of nanoscale-confined polaritons in a low-loss natural medium

Enrique Terán García
Gonzalo Álvarez Pérez[1,2], J. Duan[1,2], J. Taboada-Gutiérrez[1,2], Q. Ou[3], E. Nikulina[4], S. Liu[5], J. H. Edgar[5], Q. Bao[3,6], V. Giannini[7,8,9], R. Hillenbrand[4, 10], J. Martín-Sánchez[1,2], A. Y. Nikitin[10,11], P. Alonso-González[1,2]
[1]*Department of Physics, University of Oviedo, Oviedo 33006, Spain.*
[2]*Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo), El Entrego 33940, Spain.*
[3]*Department of Materials Science and Engineering and ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET), Monash University, Clayton, Victoria, Australia.*
[4]*CIC nanoGUNE BRTA and Department of Electricity and Electronics, UPV/EHU, Donostia/San Sebastián 20018, Spain.*
[5]*Tim Taylor Department of Chemical Engineering, Kansas State University, Manhattan, KS 66506, USA.*
[6]*Nanjing kLight Laser Technology Co. Ltd., Nanjing 210032, China.*
[7]*Instituto de Estructura de la Materia (IEM), Consejo Superior de Investigaciones Científicas (CSIC), Serrano 121, Madrid 28006, Spain*
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[9]*Centre of Excellence ENSEMBLE3 sp. z o.o., Wolczynska 133, Warsaw, 01-919, Poland.*
[10]*IKERBASQUE, Basque Foundation for Science, Bilbao 48013, Spain.*
[11]*Donostia International Physics Center (DIPC), Donostia/San Sebastián 20018, Spain*
gonzaloalvarez@uniovi.es

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Figures

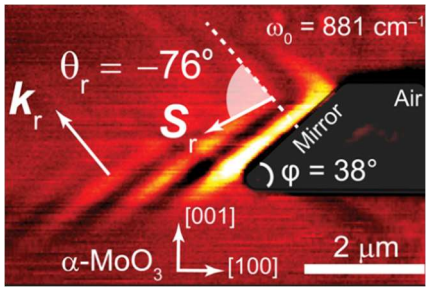

Figure 1: Visualization of negative reflection of nanoscale-confined polaritons in a natural medium.

Spin filtering induced by a magnetic insulator stripe on graphene

C H Fuentevilla[1]
J D Lejarreta[1], F Domínguez-Adame[2], E Diez[1]
[1] *Group of Nanotechnology, USAL-NANOLAB, Universidad de Salamanca, E-37008 Salamanca, Spain*
[2] *GSIC, Departamento de Física de los Materiales, Universidad Complutense, E-28040 Madrid, Spain*
chernan@usal.es

We study electronic transport properties of graphene in close proximity to a strip of a magnetic insulator, when the system is connected to nonmagnetic source and drain leads. A gate voltage creates a potential energy barrier U_0 in this region. We describe graphene electrons by means of an effective Hamiltonian [1].
The proximity exchange interaction of graphene electrons with the FMI splits the bands and open spin-dependent gaps. The band structure can be shifted upwards or downwards an amount U_0 by means of a gate voltage, what is crucial to control the spin-polarized current through the device.
The transmission coefficient is different for spin up and spin down electrons, giving rise to different spin-dependent current densities and therefore a polarization of the current density. This is a figure of merit to assess the spin-filtering properties of the device. We observe the appearance of high spin-polarization of the current density over a broad range at negative values of V_{SD}, when the density current is not small (which is desirable).
We compare the spin-polarization of the electron current calculated for several different magnetic insulators, aiming at elucidating the effects of the various model parameters on the efficiency of the devices (Figure 1). We found that those based on EuO/Gr/EuO heterostructures yield the highest efficiency [2].

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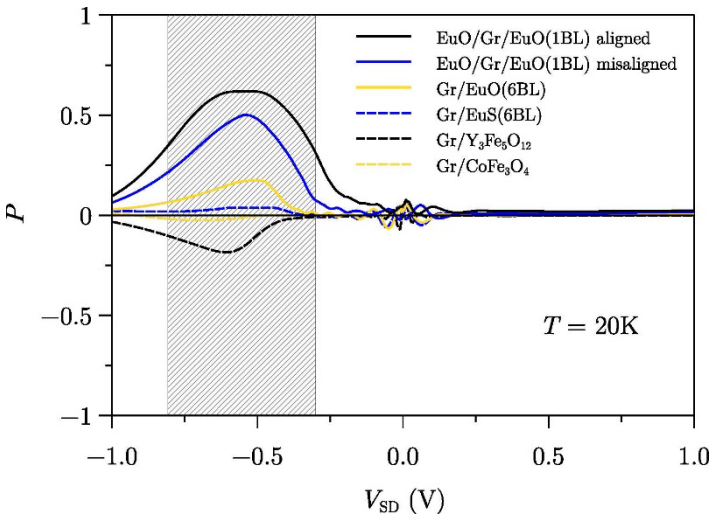

Figure 1: Current density polarization P as a function of the source-drain voltage V_{SD} for different FMI, when U_0 = 500 meV and L = 50 nm.

Structure and properties of layered materials: role of orthorhombic instability

Inés Sánchez-Movellán
José Antonio Aramburu, Pablo García-Fernández, Miguel Moreno
DCITIMAC Universidad de Cantabria, Avenida de los Castros s/n 39005, Santander, Spain
ines.sanchez@unican.es

During the last two decades a great deal of attention has been focused on layered systems containing transition metal (TM) compounds such as Cu^{2+}, Ag^{2+}, Cr^{2+}, Co^{2+} or Mn^{3+} surrounded by anions (F^-, Cl^-, O^{2-}). This trend is motivated by the discovery of a wide range of new properties and effects such as high-T_C superconducting states, 2D magnetism or semiconductor-to-metal transitions [1]. Furthermore, layered hybrid materials based on CuX_n units show fluorescence properties and play a key role in photovoltaic applications [2]. In general, this sort of systems displays low symmetries (orthorhombic, monoclinic) with MX_n distorted complexes. In the literature, these distortions have usually been ascribed to Jahn-Teller (JT) effect, discussed on the basis of simple parametrized models, which assume that the JT theory can be transferred from cubic to lower symmetries, an assumption that is, in general, mistaken [3-6].

Our study takes a different approach, based on the vibronic coupling framework [7] with a particular focus on the symmetry of the layered systems. To clarify the analysis, these systems are compared to those coming from an actual cubic structure, revealing significant differences between them. A key concept in our work is the *parent phase* [4], whose symmetry and degeneracy are directly linked to the distortion undergone by the systems. If the ground state of the MX_n units in the parent phase is non-degenerate, thus excluding the JT effect [3-6], the mechanism of symmetry breaking is the pseudo Jahn-Teller (PJT) effect. It is important to note that, despite having similar names, the physics involved in each case is entirely different [4].

The results obtained for inorganic K_2CuF_4, Rb_2CuF_4, Na_2CuF_4, Na_3MnF_6 and the hybrid $(C_2H_5NH_3)_2CdCl_4:Cu^{2+}$ layered materials [3-6] show that their parent phases are tetragonally compressed, with two equal in-plane metal-ligand distances and a shorter out-of-plane distance. In these conditions, the ground state is *non-degenerate* and therefore the driven force is the PJT effect, which elongates one of the in-plane distances. We have studied that, due to the *orthorhombic instability*, the response to pressure of these systems is highly anisotropic and can lead to switches of the main axes [5] or significant changes in the optical spectra [6].

The authors acknowledge financial support from Grant PGC2018-096955-B-C41 funded by MCIN/AEI/ 10.13039/501100011033 and by “ERDF A way of making Europe”, by the European Union. The presenting author acknowledges financial support from grant BDNS:589170 (Gobierno de Cantabria-Universidad de Cantabria)

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Electronic transport through twisted bilayer graphene flakes with defects

Pablo Moles Matías
Leonor Chico Gómez and Francisco Domínguez-Adame Acosta
GISC, Departamento de Física de Materiales, Universidad Complutense de Madrid, Pl. de las Ciencias, 1, 28040 Madrid, Spain
pmoles@ucm.es

The study of electronic transport in graphene nanoribbons and flakes aims at the design of graphene-based devices for nanoelectronics. We investigate the electronic transport properties of a twisted bilayer graphene flake contacted by two monolayer graphene nanoribbons which act as leads. The transport is governed by the interplay between the moiré pattern and the flake edges. Numerical simulations are carried out with the help of the package Kwant for quantum transport, using a tight-binding model to describe the system. The conductance and the spatial distribution of electronic states in the flake are computed. The conductance presents a strong dependence with the rotation angle between layers and is quantized for relatively large angles. In addition, we study disorder effects by adding vacancy defects to the flake, and observe its consequences on the conduction.

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Figures

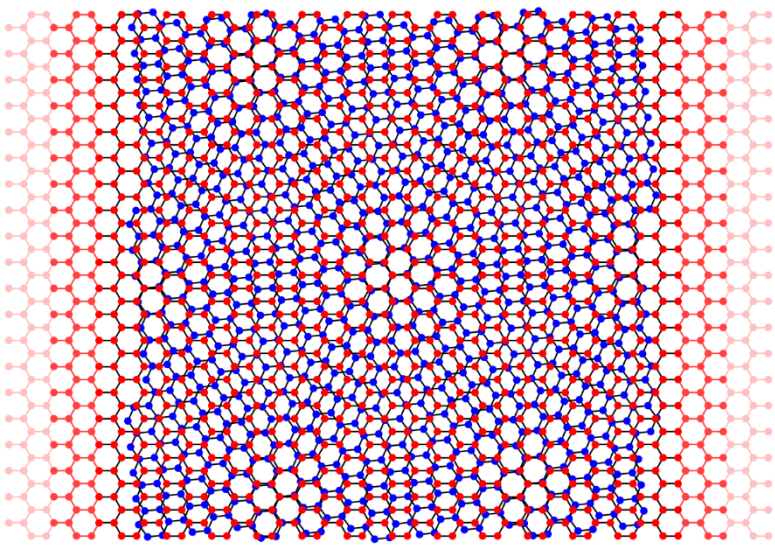

Figure 1: Twisted bilayer graphene flake contacted by two leads.

Non-perturbative indirect exchange in spin-valley coupled 2D crystals

M. R Losada[1]
A.T. Costa[2], B. Biel[1,3], J. Fernández-Rossier[2]
[1]*Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, 18071 Granada (Spain)*
[2]*International Iberian Nanotechnology (INL), Av. Mestre José Veiga, 4715-330, Braga (Portugal)*
[3]*Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071 Granada (Spain)*
mrlosada@ugr.es

In this work[1], we study indirect exchange interactions between localized spins of magnetic impurities in spin-valley coupled systems described with the Kane-Mele model. The model captures the main ingredients of the energy bands of 1H transition metal dichalcogenides (TMD) monolayers. These systems present anisotropic interactions that include Heisenberg, Ising and Dzyaloshinskii-Moriya couplings. In contrast to previous studies [2-4], we calculate the indirect exchange by using exact diagonalization of the Hamiltonian, avoiding the use of perturbation theory and the momentum cut-off. We study the interplay between the symmetry of indirect exchange (Heisenberg, Ising and DM), the Fermi-surface topology and the relative orientation between the magnetic impurities. We find that the anisotropic nature of the interaction depends on the impurities orientation. Moreover, we relate the contribution of intervalley or intravalley electronic scattering processes with the Fermi-surface topology. We also test the validity of the perturbative results and conclude that it is a good approximation beyond the expected regime. Finally, we show that the effective Hamiltonian derived from perturbation theory works in the non-perturbative regime.

The authors kindly acknowledge financial support by the Junta de Andalucía under the Programa Operativo FEDER P18-FR-4834. B.B. also acknowledges financial support from AEI under project PID2021-125604NB-I00. The Albaicín supercomputer of the University of Granada are also acknowledged for providing computational time and facilities.

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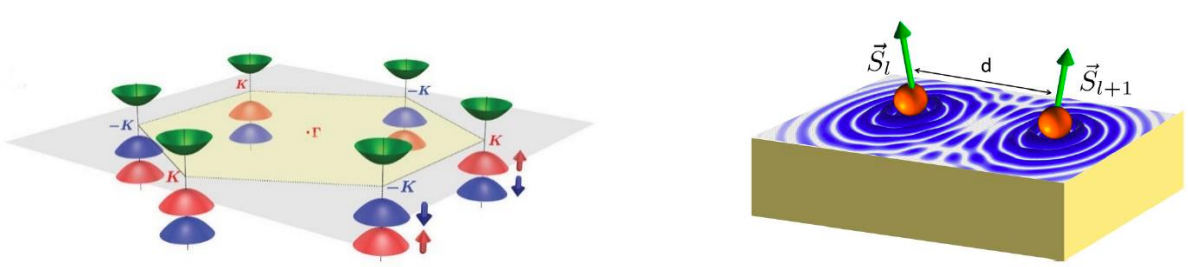


(a) (b)

Figure 1: (a) Schematic drawing of the spin-valley coupled band structure (Picture taken from [5]). (b) Scheme of the mechanism of the indirect exchange interaction between two localized surface spins (Taken from [6])

Dynamic stability and magnetism of David star charge density waves in transition metal dichalcogenide systems

Jan Phillips[1,2]
Adolfo O. Fumega[3], Víctor Pardo[1,2]
[1] *Departamento de Física Aplicada - Universidade de Santiago de Compostela, 15782 Campus Sur s/n, Santiago de Compostela, Spain.*
[2] *Instituto de Materiais (iMATUS) - Universidade de Santiago de Compostela, 15706 Campus Sur s/n, Santiago de Compostela, Spain.*
[3] *Department of Applied Physics – Aalto University, 02150, Espoo, Finland.*
j.phillips@usc.es

Monolayer group V transition metal dichalcogenides in their 1T phase have recently emerged as a platform to investigate rich phases of matter resulting from strong electron correlations. The magnetism of these systems interplays with different ordered phases, such as charge density waves (CDW). In particular, the so-called David star (Figure 1) CDW phase (with a $\sqrt{13}\times\sqrt{13}$ reconstruction) that might arise in these systems leads to the emergence of a spin 1/2 per David star, which has been discussed in the framework of spin liquids. In this talk, we present ab initio calculations based on the density functional theory for different V-, Nb-, and Ta-based chalcogenides where we study the band structure, density of states, and phonon spectra of various of these compounds in the $\sqrt{13}\times\sqrt{13}$ cell. By doing this, we obtain information about the possible charge-density-wave q-vectors that may be responsible for the appearing instabilities, if these exist, and the flat bands that emerge in this kind of system as a function of correlations and stoichiometry.

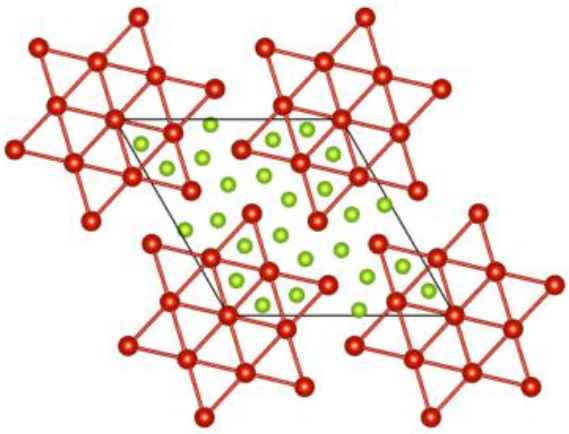
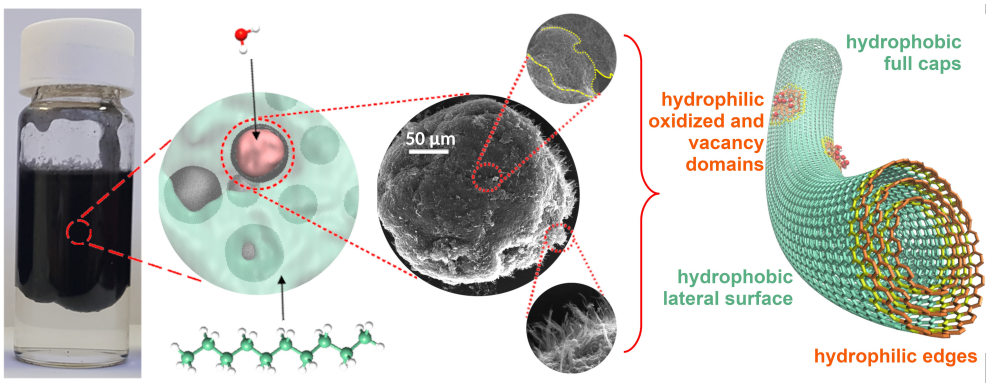


Figure 1: David star CDW phase for a transition metal dichalcogenide. The transition metal atoms are represented in red, while the chalcogene atoms are represented in green.

The Origin of Amphiphatic Nature of Short and Thin Pristine Carbon Nanotubes - a Fully Recyclable 1D Emulsion Stabilizers

Karolina Z. Milowska[1,2,3]
Anna W. Blacha[4], Mike C. Payne[3], Heather F. Greer[5], Artur P. Terzyk[6], Emil Korczeniewski[6], Aleksandra Cyganiuk[6], Sławomir Boncel[4]
[1] *CIC nanoGUNE, Donostia-San Sebastián, Spain*
[2] *Ikerbasque, Basque Foundation for Science, 48013, Bilbao, Spain*
[3] *TCM Group, Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom*
[4] *Faculty of Chemistry, Silesian University of Technology, Gliwice, Poland*
[5] *Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, United Kingdom*
[6] *Physicochemistry of Carbon Materials Research Group, Faculty of Chemistry, Nicolaus Copernicus University, Toruń, Poland*
kz.milowska@nanogune.eu

Carbon nanotubes (CNT)s have already demonstrated scientific and technological breakthroughs including scalable coatings, composites, supercapacitors, tissue engineering, and biosensors. However, inconsistencies in understanding of water-solid interfaces for realistic CNTs hamper their individualization-driven functionalities, processability in benign media, and compatibility with a broad-scale of matrices. Pristine CNT processing based on water and inexpensive *n*-alkanes within a low energy regime would constitute an important step towards greener technologies. Therefore, we quantitatively assess structural CNT components, placing various CNTs on the scale from hydrophobicity to hydrophilicity. This structural interweave can lead to amphipathicity enabling the formation of water-in-oil emulsions. Combining experiments with theoretical studies, we comprehensively characterize CNTs and CNT emulsions establishing descriptors of the emulsifying behavior of pristine and purified CNTs. They emerge as having hydrophilic open-ends, small number of oxygen-functionalized/vacancy surface areas, and hydrophobic sidewalls and full caps. The interplay of these regions allows short and thin CNTs to be utilized as fully recyclable 1D surfactants stabilizing water/oil emulsions which, as we demonstrate, can be applied as paints for flexible conductive coatings. These coatings are characterized by considerable smaller resistance than coatings with additional surfactants or containing pristine graphene. In addition, we show how the amphipathic strength depends on CNT size, the pristine-to-oxidized/vacancy domains and the oil-to-water ratios. Our results confirm shorter and thinner pristine multi-walled CNTs as promising candidates for fully recyclable 1D emulsifying agents capable of replacing aquatoxic low-molecular surfactants in the the preparation of composites, in/as heat transfer (io)nanofluids, superlubricants, paints, coatings, electrocatalysts and as drug vehicles for locoregional therapy or contrast agents in bioimaging.



Van der Waals Epitaxy and properties of GaSe and InSe superlattices

Marcel S. Claro*[1,2]
Khalil El hajraoui[1] , Justyna Grzonka[1], Juan P. Martínez-Pastor[3], Alejandro Molina-Sánchez[3], David Fuertes Marrón[4], Paulo J. Ferreira[1], Sascha Sadewasser[1]
[1] *International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga, 4715-330, Braga, Portugal*
[2] *Centro Singular de Investigación en Química Biológica y Materiales Moleculares (CIQUS), Universidade de Santiago de Compostela, C/ Jenaro de la Fuente s/n ,15782, Santiago de Compostela, Spain*
[3] *Instituto de Ciencia de Materiales, Universidad de Valencia, P.O. Box 22085, 46071 Valencia, Spain*
[4] *Instituto de Energía Solar-ETSIT, Universidad Politécnica de Madrid, 28040, Madrid, Spain*
*marcel.santos@usc.es

Two-dimensional (2D) semiconductors GaSe and InSe belong to the group of layered III-VI post-transition metal chalcogenides (PTMC). This new class of 2D materials has great potential for optoelectronic applications in the form of atomically thin films due to their exceptional optical and transport properties that usually cannot be found in bulk semiconductor materials, such as high electron mobility, quantum Hall effect and anomalous optical response. Recently, it was demonstrated that heterostructures from InSe and GaSe flakes exhibit optical transitions that densely cover the spectrum from violet to infrared, which is hard to achieve in any other semiconductor materials system[1].
In this work, we present pioneering work on van der Waals epitaxy of GaSe/InSe heterostructures, capable of producing quantum wells and superlattices on different substrates which exhibit photoluminescence (PL) and absorption in confined states. Proposed theoretical models and comparison with experimental PL data are shown. We also discuss the different polytypes and polymorphs of GaSe and InSe and the strain in these films[2]. Properties are calculated by Density Functional Theory (DFT) and it shows that Mexican-hat valence bands are present even on thick films of InSe/GaSe type-II heterostructures, resulting in 50% enhancement on thermoelectric figure-of-merit zT at room-temperature when compared with bulk InSe[3].

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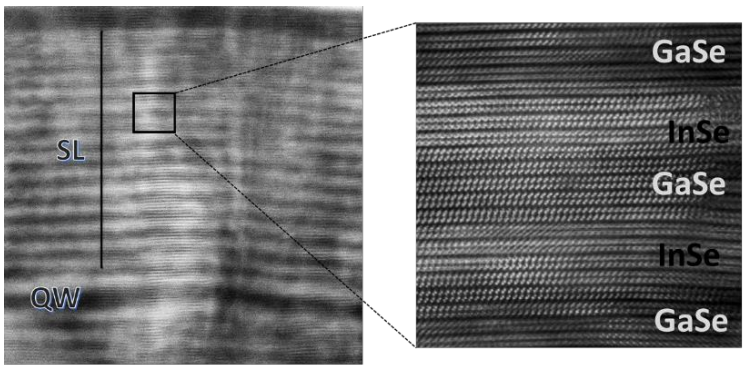

Figure 1: Cross-sectional view by Transmission Electron Microscopy (TEM) of 2.5nm GaSe/ 2.5nm InSe superlattice(in detail) embedding a quantum-well (on Sapphire substrate).

Phase engineering of two-dimensional Transition Metal Ditellurides

Joan Ripoll Sau[1,2]
I. Di Bernardo[2], F. Calleja[1], P. Casado Aguilar[1,2], I.M. Ibarburu[1,2], R. Miranda[1,2,3,4], A.L. Vázquez de Parga[1,2,3,4], M. Garnica[1,3]
[1]*Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), 28049 Madrid, Spain*
[2]*Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain*
[3]*Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, 28049 Madrid, Spain*
[4]*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain*
joan.ripoll@imdea.org

Phase engineering of two-dimensional transition metal ditellurides (2D-TMDTs) is a promising way to exploit their electronic properties in order to apply them in electronic devices such as photodetectors, LEDs, phototransistors, and solar cells [1]. 2D-TMDTs have a MTe_2 stoichiometry, where M is a transition metal (groups IV-X). Interestingly, their properties change according to the transition metal, the crystallographic structure and number of layers. An interesting example is $MoTe_2$, which presents a semiconducting hexagonal phase showing an indirect bandgap in bulk (2H phase) or a direct bandgap at the monolayer (1H) [2] or the semimetallic distorted octahedral (1T′) phase (unstable in bulk) predicted to exhibit quantum spin Hall (QSH) effect in the monolayer regime [3]. Another example is $TaTe_2$, which in bulk is only stable in the 1T' distorted octahedral phase [4] but is predicted to exhibit two additional metallic phases in the ML: one magnetic (1H) and the other non-magnetic (1T) [5]. Here, we report the growth of 2D islands of $MoTe_2$ and $TaTe_2$ via molecular beam epitaxy (MBE) on epitaxial graphene on Ir(111) (Fig. 1(a)). We show how by varying the growth parameters, such as substrate temperature (Fig. 1(b) and 1(e)) and precursor ratio, we can tune the relative coverage of different phases. Their structural and electronic characteristics are studied by means of scanning tunneling microscopy (STM).

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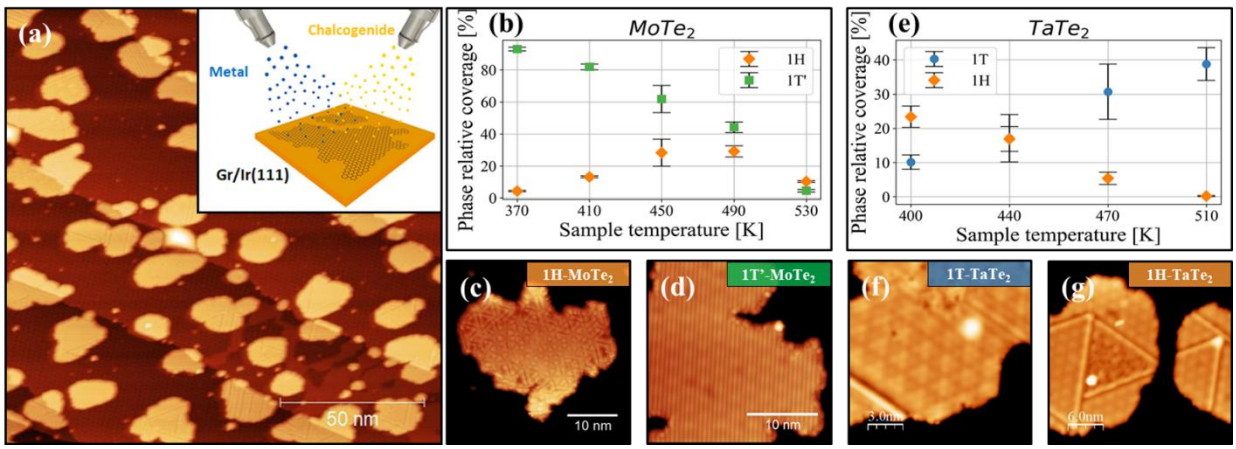

Figure 1: (a) Large STM image of $TaTe_2$ islands on gr/Ir(111) (V = -1V; I = 0.1nA). Inset: sketch of the growth procedure. (b) Relative coverage of 1T' vs. 1H-$MoTe_2$ phases for different growth temperatures. STM images of (c) 1H-$MoTe_2$ (V = 0.5V; I = 0.1nA) and (d) 1T'-$MoTe_2$ islands (V = 1V; I = 0.1nA). (e) Relative coverage of 1T vs 1H-$TaTe_2$ phases for different growth temperatures. STM images of (f) 1T-$TaTe_2$ (V = 0.75V; I = 0.2nA) and (g) 1H-$TaTe_2$ islands (V = 1V; I = 0.2nA).

Local and non-local transport of composite Fermions in graphene Moiré superlattices

Vittorio Bellani[1]
Juan Salvador-Sánchez[2], Ana Pérez Rodriguez[2], Oleksandr Zheliuk[3], Uli Zeitler[3], Enrique Diez[2], and Mario Amado[2]
[1]*Department of Physics and INFN, University of Pavia, Italy*
[2]*Nanotechnology Group, Department of Fundamental Physics, University of Salamanca, Spain*
[3]*High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, The Netherlands*
bellani@unipv.it

Recent quantum Hall experimental investigation on graphene Moiré superlattices shows non-local currents with unexpected behavior. We therefore studied the quantum Hall states in the integer and fraction regimes, in the graphene Moiré superlattices created by near 180-degree misalignments, at magnetic fields up to 30 T [1]. The sample with well-developed Moiré superlattices at voltages around ± 10 V, and mobility 250.000 $m^2V^{-1}s^{-1}$, show at $\nu > 1$ the fractional states at the odd denominator $\nu = p/3$ fillings 5/3, 11/3, 14/3, 16/3 in R_{xx} and R_{xy} resistivities and in the non-local transport. We have been able to identify the fractional states for composite Fermions (CF) with small filling factors and higher order composite fermion states, which are present at the highest fields. At $\nu < 1$ we observed the $\nu = 2/3$ state, which edge transport nature is still now understood, and was originally proposed to host counter-propagating modes with different filling. The non-local transport, both in the integer and fractional regimes, measured as a function of the electron and hole density, shows mirror reflection symmetries for positive and negative magnetic field, which give information on the edge and counter-propagating modes and is linked to CF correlations in the compressible-incompressible fluid [2].

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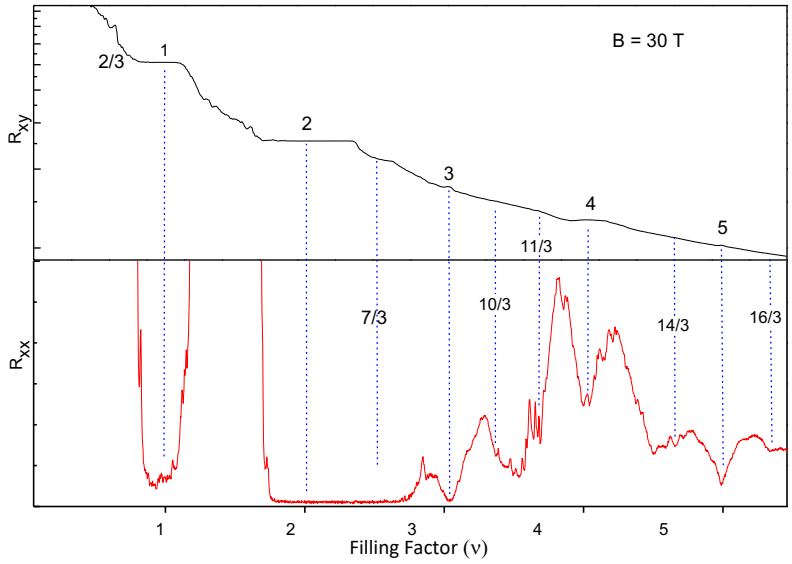


Figure 1: Integer quantum Hall states and composite Fermions in the Moiré landscape.

Synthesis and characterization of hybrids materials of transition metal oxides and graphene oxide. Evaluation of their properties as CO_2 adsorbents and as supercapacitor electrodes

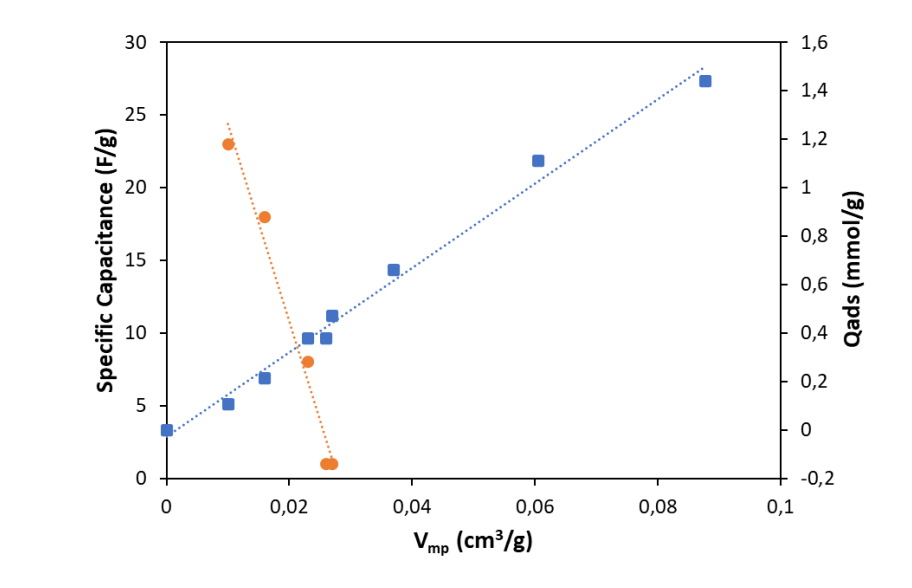
M. Dolores Merchán[1]
Luis Fernández-Gallego[1], Víctor Fernández-Jiménez[1], Santiago Bernardi[2], Alejandra García Gómez[2], David López-Díaz[1], M. Jesús Sánchez Montero[1] and M. Mercedes Velázquez[1]
[1]*Nanotechnology group, Department of Physical Chemistry, University of Salamanca, E37008 Spain*
[2]*Gnanomat S.L. E28049 Madrid, Spain*
mdm@usal.es

Graphene-based hybrid materials have been prepared by incorporating inorganic species and/or cross-linking of organic species through covalent and/or noncovalent interactions. These graphene-based hybrid materials show improved or excellent performance in various fields such as catalysts, electrode materials, solar cells for hydrogen storage, etc.

In previous works [1-2], we have studied the capacity of hybrid materials that combine graphene oxide with polyaniline and with magnetite to retain CO_2 and it has been found that the capacity increases linearly with increasing the volume of micropores of the material. At this work an attempt has been made to increase the microporosity with transition metal oxides MnO_2, ZnO and SnO_2 with different (GO/Metal oxide ratio) with the tentative of increasing the microporosity.

These materials have been characterized by XRD, TEM, XPS and by gas adsorption measurements N_2 and CO_2. Since these materials could present the capacitance due to the EDLC double layer provided by carbonaceous materials and the pseudocapacitative properties of metal oxides, the measurement of specific capacitance (SC) in 3-electrode electrochemical cells using KOH as electrolyte has been analysed.

We have found that the capacity of adsorption of CO_2 of hybrids is higher than the value of graphene oxides and increases with the micropore volume while the specific capacitance decreases as the micropore volume increases.



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Dynamic light scattering applied to soft systems out of thermal equilibrium

José López-Molina
Ana Belén Jódar Reyes, Irene Adroher Benítez, José Manuel Peula García, Arturo Moncho Jordá, María Tirado Miranda
Grupo de Física de Fluidos y Biocoloides, Facultad de Ciencias, Avda. Fuentenueva s/n, Granada (España)
josel@ugr.es, mtirado@ugr.es

In Colloid Physics, the technique known as dynamic light scattering (DLS) consists of the analysis over time of the fluctuations of scattered light that come from a colloidal particle. The particle geometry and size, the particle motion within the collectivity (particle interactions) and the suspension medium mechanical properties are directly related to these fluctuations. Therefore, DLS is an excellent method for particle size determination in dilute systems with monodisperse uniform spheres and under thermal equilibrium. However, the temporal correlations in the scattered light fluctuations by some complex systems show experimentally a behaviour far from theoretical predictions if a temperature gradient is applied. In particular, thermoresponsive-microgels can develop anomalous correlations for determined experimental conditions. These highlights show the need to extend DLS theory to explain the new complex behaviour of these real systems.

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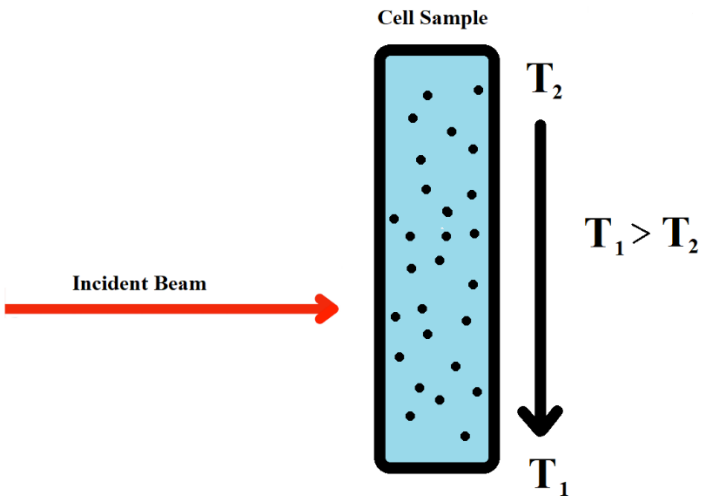

Figure 1: Schematic representation of the DLS experiment under a temperature gradient. The sample cell is subjected to a temperature difference between its base and its top.

Method of Rapid Prototyping of Paper-based Devices using Solution-Processable Nanomaterials

Gulsum Ersu[1]
Sruthi.Kuriakose[1], Yigit Sozen[1], Estrella Sánchez[1], Carmen Munuera[1], Beatriz H. Juárez[1], Federico Mompean[1], Mar Garcia Hernandez[1], Ferry Prins[2], Joshua O. Island[3], Andres Castellanos-Gomez[1]

[1]Materials Science Factory. Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, E-28049, Spain
[2]Condensed Matter Physics Center (IFIMAC) and Department of Condensed Matter Physics, Autonomous University of Madrid, 28049 Madrid, Spain
[3]Department of Physics and Astronomy, University of Nevada Las Vegas, Las Vegas, NV, 89154, USA
gulsumersu@gmail.com, andres.castellanos@csic.es

The development of solution-processible organic semiconductors in the 2000s unleashed the opportunity to apply all the ink-printing lithographic techniques, optimized over the last centuries, to fabricate electronic devices. The combination of solution-processable nanomaterials and ink-printing techniques can be crucial to developing ultra-low-cost electronic components for the incipient field of ubiquitous electronics. The most widespread ink-printing lithography methods for the fabrication of devices (inkjet printing and spray-coating), however, require rather sophisticated and expensive equipment making the entry-level threshold too high to start producing ink-printing-based devices in many laboratories. This is in striking contrast with the unprecedented low threshold to produce electronic inks with certain nanomaterials that can be easily carried out in labs running under a low budget.
Motivated by this background, we aimed to develop a low-cost, easy and robust technique to print solution-processible inks to allow rapid device prototyping for researchers developing inks of nanomaterials. We have tested this method to print inks of many different materials (quantum dots, hybrid perovskites, organic semiconductors, van der Waals materials, with very different electronic properties (ranging from insulators to superconductors) on paper substrates. We illustrate the use of this technique and tools with different application examples: Printing an invisible QR code, coating a paper substrate with a film of high critical temperature superconductor, and fabricating a paper-supported photodetector device.

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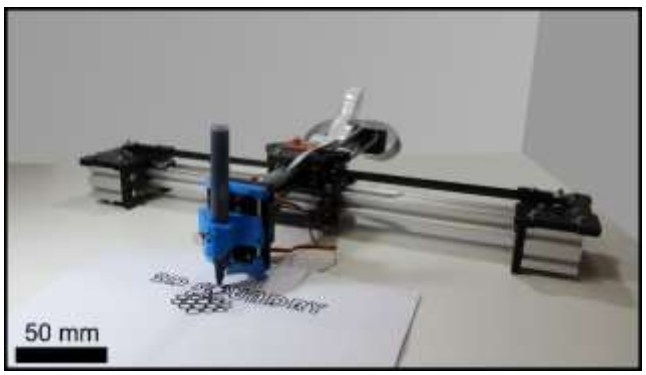

Figure 1: Digital photograph of the equipment used for printing

High-mobility MoS_2 phototransistor using biodegradable albumen dielectrics

Thomas Pucher[1]
Yong Xie[1], Pablo Bastante[2] and Andrés Castellanos Gómez[1]
[1] *Materials Science Institute, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), 28049, Madrid, Spain*
[2] *Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049, Madrid, Spain*
thomas.pucher@csic.es

This work demonstrates the fabrication and characterization of performance-enhanced phototransistors by combining cheap, biodegradable and natural chicken eggwhite dielectrics with transition metal dichalcogenide materials, as MoS_2, paving the way for biocompatible two-dimensional material optoelectronic devices. As it has been shown in other works, eggwhite can be used as dielectric for various nanoelectronic applications [1,2]. By introducing albumen as an insulator to fabricate few-layer MoS_2 transistors and photodetector devices, high carrier mobilities (up to 300 cm^2/Vs) and on/off current ratios (>10^4) are observed. The developed phototransistor exhibits high switching currents and good photoresponsivity at low gate voltages. Fast switching speeds are realized in photoconductivity mode (50ms). The fabricated devices show high stability and reproducibility in ambient atmosphere and improved transfer characteristics at vacuum conditions. Eggwhite dielectrics offer a cost-effective bio-alternative to conventional SiO_2-dielectrics [1]. The albumen dielectric layer is created by a basic spin coating technique and MoS_2 is introduced by deterministic transfer [3]. This work shows that not only the fabrication and combination with 2D materials is simple, but additionally performance characteristics are improved significantly compared to their SiO_2 counterpart [4]. The presented study reveals for the first time the combination of chicken egg albumen with two-dimensional materials for optoelectronic device applications.

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Figures

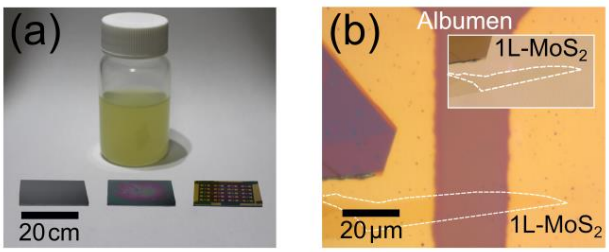

Figure 1. (a) Fabrication steps; (b) Microscope image of fabricated 1L-MoS_2 albumen transistor

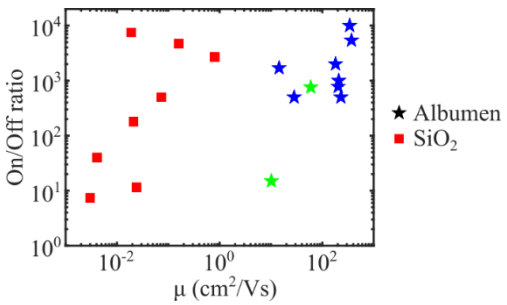

Figure 2. Mobility vs On/Off ratio. Comparison between standard SiO_2 devices and albumen devices

Electronic and ionic conduction in biomaterials based on engineered proteins

M. Reyes Calvo[1,2], Lisa Almonte[1], Juan David Cortés[1], Carlos Sabater[1], Aitziber López-Cortajarena[3,4]
[1]*Departamento de Física Aplicada – Universidad de Alicante, Alicante, Spain*
[2]*Instituto Universitario de Materiales IUMA, Universidad de Alicante, Alicante, Spain*
[3]*CIC biomaGUNE, BRTA, Donostia-San Sebastián, Spain*
[4]*Ikerbasque, Basque Foundation for Science, Bilbao, Spain*
reyes.calvo@ua.es

https://www.e-prot.com/

Proteins, the building blocks of living systems, offer structural stability and inherent biocompatibility and sustainability for biomaterial fabrication. In terms of their conductivity, despite being a scarce phenomenon, nature provides fascinating examples for extremely effective extracellular long-range electron transfer and for intrinsic protonic conduction, such as protein nanowires found in sediment bacteria, and cephalopod structural proteins, respectively. Fueled by their attractive properties, and new insights from structural biology into the basis of their promising conductive properties, the past few years have seen rapid growth in the study of conductive peptide and protein- based assemblies. However, the generation of electron or proton conductive biomolecular systems has not been tackled from a rational protein design perspective.

In this work, we study conduction in films made of self-assembled modular consensus tetratricopeptide repeat (CTPR) protein.[1] This robust protein scaffold remains intact during the protein engineering and sequence optimization process aiming at improving their conductivity, while allowing the control of the stability and properties of the final materials. Our experiments show that CTPR-based biomaterials exhibit strong ionic conductivity without mechanical integrity loss thus demonstrating the intrinsic potential of these proteins for the development of artificial conductive proteins. A detailed study of electronic and ionic contributions to conductivity is key to optimize their properties towards different applications in energy storage or bioelectronic devices.

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Unveiling the structural and optical properties of anisotropic hybrid Bi_2S_3@Au nanocomposites

José Alejandro Ruiz-Torres
M. Escoda-Torroella[1,2], C. Moya[1,2], A. Fraile Rodríguez[1,2], A. Labarta[1,2], and X. Batlle[1,2]
[1]*Departament de Física de la Matèria Condensada, Martí i Franquès 1, 08028 Barcelona, Spain,*
[2]*Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, 08028 Barcelona, Spain*
jruiz-torres@ub.edu

Theragnostic nanoparticles are multifunctional nanosystems that combine diagnostic and therapeutic capabilities into one single agent [1]. Although numerous types of theragnostic nanoparticles, both organic and inorganic, have been developed in the last decade for treating cancer, there is still a big gap between fundamental and applied research. In this regard, hybrid Bi_2S_3@Au nanocomposites have been drawing much attention due to their superior performance in both computed tomography and photothermal therapy. In this work, we have advanced in this field by designing anisotropic hybrid Bi_2S_3@Au nanocomposites with a modulated shape, Au content, and surface functionalization in three steps. First, 35 nm-Bi_2S_3 nanorods with widths ranging from 6 to 12 nm were synthesized by the hot injection of thioacetamide on a Bi (III) neodecanoate solution [2]. Second, satellite Au nanoparticles were grown onto the Bi_2S_3 surface by the controlled reduction of Au (III) tetrachloride in presence of oleylamine in mild conditions. UV-vis spectra of samples reveal significant changes in the optical absorption as a function of the nanocomposite shape and Au content. The thicker Bi_2S_3 nanorods show, for example, greater absorption in the near-infrared region, probably due to the decrease in the quantum confinement along the short-axis direction, while the hybrid Bi_2S_3@Au nanocomposites show a larger enhancement throughout the UV-vis region possibly induced by the Au content. Finally, the anisotropic hybrid Bi_2S_3@Au nanocomposites were transferred from an organic solvent to water by the grafting of PEG-thiolate ligands onto the nanocomposite surface. The as-prepared samples show good stability in water and in phosphate buffer solution.

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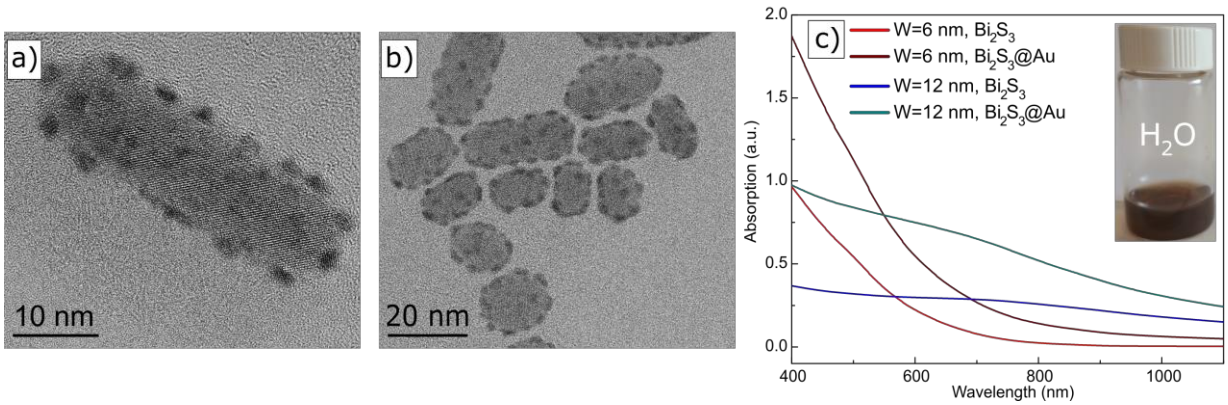

Figure 1: a) Rod-like Bi_2S_3@Au, b) Ellipsoidal-like Bi_2S_3@Au, and c) UV-vis spectra of samples with and without Au, with an image of a Bi_2S_3@Au sample stable in water. W stands for the width of the nanoparticles.

Performing 3DDLS to study the dynamics of dense microgel suspensions

A. Arenas-Gullo[1,2]
A. Fernández-Nieves[1,2,3]
[1]*Department of Condensed Matter Physics, University of Barcelona, 08028 Barcelona, Spain*
[2]*Institute for Complex Systems (UBICS), University of Barcelona, 08028 Barcelona, Spain*
[3]*ICREA-Instituci´o Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain*
adrianarenasgullo@ub.edu

The dynamics of a microgel suspension is highly influenced by its particle concentration. We are using a 3DDLS setup to perform experiments with temperature sensitive colloidal hydrogels. The (lag time) correlation function shows that for low values of the generalized volume fraction, ζ, the relaxation takes place exponentially. However, increasing ζ leads to a stretched exponential behaviour. The structural relaxation time, τ_α, corresponding to the long time decay, increases significantly and then seems to reach a plateau. This behaviour indicates the system could remain supercooled and exhibit a relaxation at constant τ_α, due to particle shrinkage, or be a colloidal glass that undergoes non equilibrium dynamics known as aging. To adress this question, we aim to study some other variables, such as the dynamical susceptibility $\chi(\tau_\alpha)$, at different concentrations.

Charge-Transfer Complex Formation in Organic Semiconductor Films and its role in Surface Doping

Alba Cazorla[1], Adara Babuji[1], Eduardo Solano[2], Carmen Ocal[1]*, Esther Barrena[1]*,
[1]*Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), 08193 Bellaterra, Barcelona, Spain*
[2] *ALBA Synchrotron, 08290 Cerdanyola del Vallès, Barcelona, Spain*
Email: e.barrena@csic.es

Among the vast number of organic semiconductors (OSCs) developed in the last decades, [1]benzothieno [3,2-b]benzothiophene (BTBT) derivatives have emerged as one of the best performing materials for p-type organic field-effect transistors (OFETS). Understanding and controlling molecular doping as a versatile platform for tuning the optoelectric properties of OSCs, still remain a challenge for further advancements in organic electronics. Contact and channel doping, generally referred as surface doping, are two general approaches used to improve OFETs operation, which rely on integer electron charge transfer between the OSC and the dopant. In this work, we address the structural properties of BTBT films during the deposition of a p-type dopant, 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F_6TCNNQ), with special attention to the comparison of two BTBT derivatives, namely 2,7-dioctyl-BTBT (C_8-BTBT-C_8) and 2,7-diphenyl-BTBT (DPh-BTBT). Grazing incidence wide-angle X-ray scattering (GIWAXS) was performed in the course of thermal annealing of the films. Although both BTBT-based films are isostructural, we find important structural differences upon the deposition of F_6TCNNQ. The deposition of F_6TCNNQ on C_8-BTBT-C_8 results on the formation of a co-crystalline mixed phase at the interface with charge-transfer complex (CTC) properties (Figure 1), which is further promoted by thermal annealing [1]. We demonstrate the key role of the formed charge transfer complex in surface doping for improving channel field-effect mobility and reducing the threshold voltage in organic field-effect transistors. In contrast, F_6TCNNQ on DPh-BTBT results in a planar heterostructure, without intermixing of both molecules.

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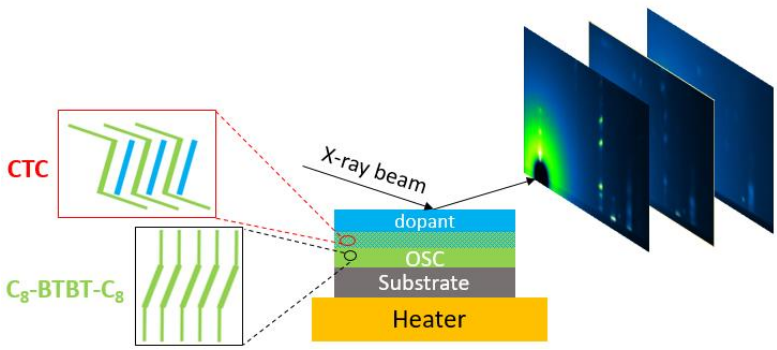

Figure 1. Sketch illustrating the structural changes upon thermal annealing for F_6TCNNQ (dopant) on C_8-BTBT-C_8 (OSC).

Percolating Superconductivity in Air-Stable Organic-Ion Intercalated MoS_2

Jose M. Pereira[1]

Daniel Tezze[1], Iris Niehues[1], Yaiza Asensio[1], Haozhe Yang[1], Lars Mester[1,2], Shu Chen[1], Felix Casanova[1,3], Alexander M. Bittner[1,3], Maider Ormaza[4], Frederik Schiller[5], Beatriz Martín-García[1,3], Rainer Hillenbrand[1,3], Luis E. Hueso[1,3], Marco Gobbi[1,3,5]

(1) *CIC nanoGUNE BRTA, Tolosa Hiribidea 76, 20018, Donostia, Spain.*
(2) *Attocube Systems AG, Eglfinger Weg 2, 85540, Haar, Germany.*
(3) *IKERBASQUE Basque Foundation for Science, Euskadi Plaza 5, 48009, Bilbao, Spain.*
(4) *Departamento de Polímeros y Materiales Avanzados: Física, Química y Tecnología, Facultad de Químicas UPV/EHU, Apartado 1072, 20080, Donostia, Spain*
(5) *Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, Paseo de Manuel Lardizabal 5, 20018, Donostia, Spain.*

j.pereira@nanogune.eu

When doped into a certain range of charge carrier concentrations, MoS_2 becomes a degenerate semiconductor characterized by exotic phenomena such as charge density waves (CDWs) or superconductivity.[1] Typically, this carrier concentration doping level is achieved via ionic-liquid gating or alkali-ion intercalation.[2,3] Here, we report the first observation of superconductivity and a CDW state emerging in organic-ion intercalated MoS_2. Our results indicate that these correlated electronic phases depend dramatically on the intercalated cation, demonstrating the potential of organic ion intercalation to finely tune the properties of 2D materials. Moreover, we observe that a fully developed zero-resistance state is exclusive of bulk samples, which we understand as the evidence of the presence of 3D superconductive paths that are severed once the crystals are mechanically exfoliated. Our results establish organic-ion intercalated MoS_2 as a platform to study the emergence and modulation of correlated electronic phases.[4]

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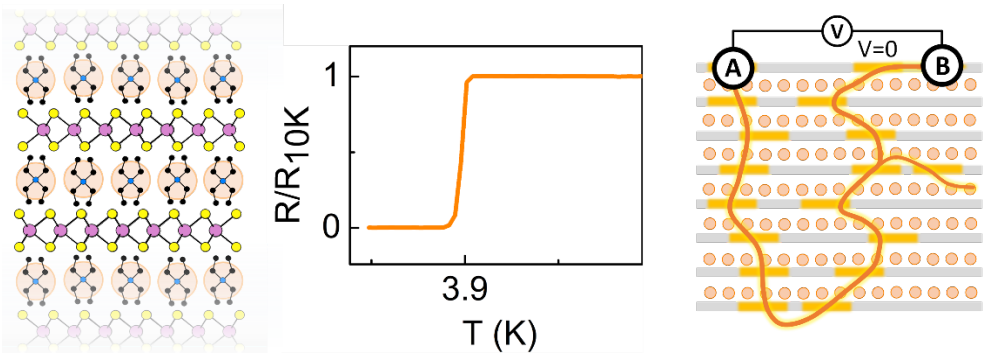

Figure 1: The intercalation of TEA^+ cations in MoS_2 leads to the emergence of superconductivity in the bulk due to the formation of percolating path resulting from the alignment of nanoscale-sized highly-doped regions located in contiguous layers.

Strong coupling for spin clock states in electronuclear spin qudits based on vanadyl porphyrin molecules

Ignacio Gimeno Alonso[1]
Ainhoa Urtizberea[1,2], Juan Román-Roche[1], David Zueco[1], Agustín Camón[1], Pablo J. Alonso[1], Olivier Roubeau[1], Fernando Luis[1]
[1]*Instituto de Nanociencia y Materiales de Aragón, CSIC and Universidad de Zaragoza, c/ Pedro Cerbuna, 12, 50009 Zaragoza, Spain*
[2]*Centro Universitario de la Defensa, Carretera de Huesca s/n, 50090 Zaragoza, Spain*
ngimeno@unizar.es

The possibility of encoding several qubits in vanadyl porphyrin molecules hosting a S = 1/2 electronic spin coupled to a I = 7/2 nuclear spin has been explored. A complete study of the spin Hamiltonian and the spin dynamics has been performed via a combination of electron paramagnetic resonance, heat capacity, magnetization and on-chip magnetic spectroscopy experiments performed on single crystals, observing several properties that make each molecule fulfil the conditions to act as a universal 4-qubit processor or, equivalently, as a d = 16 qudit in the low field region (B < 0.1 T). In this region, the combined effect of Zeeman and hyperfine interactions gives rise to a set of anticrossings between the electronuclear spin states. In these anticrossings, known as spin-clock transitions, the system becomes almost insensitive to fluctuations of the magnetic field, making the spin coherence time T_2 maximum.[1] At the same time, the overlap between the spin states involved in the transition becomes maximum, being possible to increase the spin-photon coupling G without the cost of increasing decoherence. Here, we show the possibility of achieving the strong coupling regime ($G > \gamma \sim T_2^{-1}$) close to the clock transitions that take place in molecular crystals formed by these vanadyl porphyrin molecules. An analysis of these transitions via on-chip magnetic spectroscopy has been performed using concentrated and diluted crystals, determining the evolution of the spin-photon coupling as we move away from the level anticrossings.

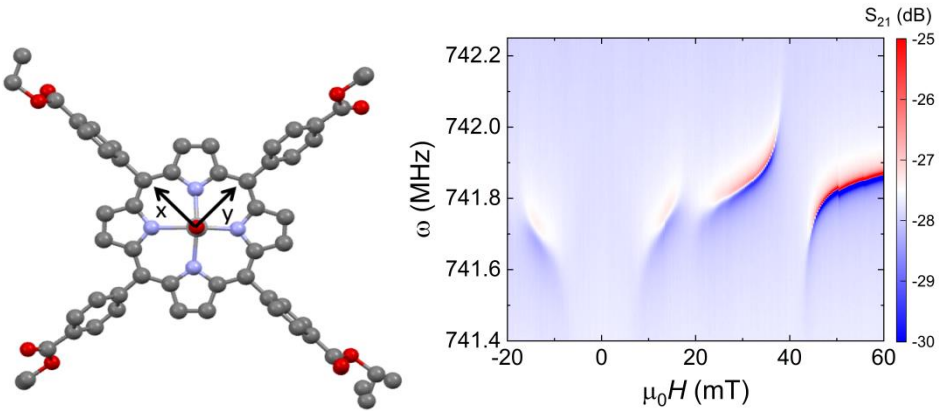

Figure 1: (Left) top view of the vanadyl porphyrin molecule, showing the vanadyl group at its centre. (Right) 2D plot of the microwave transmission of a resonator coupled to a crystal made up of these vanadyl molecules. The transitions observed at zero field and 20 mT are close to the energy minima of two clock transitions.

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Modelling and optimization of perovskite/perovskite tandem solar cells through plasmonic effects

Jaime Bueno Benito[1*]
Sol Carretero-Palacios[1], Miguel Anaya[2]
1. Dpt. Física de Materiales, Instituto de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, 28049-Madrid, Spain
2.Department of Chemical Engineering & Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS, UK
Email: jaime.buenob@estudiante.uam.es

Over the last decade, halide perovskites have irrupted as a game changer for the demonstration of highly efficient emerging optoelectronic devices. Their outstanding properties and ease of processing have allowed a meteoric rise in efficiencies, surpassing 25% in single junction solar cells. Although these performances bring them to the level of matured technologies such as silicon PV, they are fundamentally limited by thermodynamic limits, as described by the Shockley-Queisser model.[1] Recently, perovskite/perovskite tandem solar cells have been demonstrated as true candidates to deploy a third-generation PV technology with unrivalled performances.[2,3] However, they are still lagging behind their theoretical ceilings due to the inefficient harvesting of light occurring at the alloyed Pb/Sn perovskite, lowgap subcell.

In this talk, we introduce how nanoplasmonic structures embedded in lowgap perovskite films have the potential to dramatically boost the efficiency of perovskite tandem solar cells. We present a comprehensive analysis of the optical constants reported in the literature for this family of semiconductors, finding significant variations even for materials with the same nominal composition. Taking advantage of Kramers-Kronig consistent refractive indices, we perform advanced FDTD based calculations to evaluate the effect of plasmonic structures in the absorption of Pb/Sn perovskites. In particular, we screen a multiparametric space including different types of metals (e.g. Ag, Au, Al, etc.), particle sizes and volume filling fraction with the aim of maximising light harvesting while minimising parasitic absorption. We show how a fine balance between the perovskite properties and the near field plasmonic effects results in dramatic increases in the calculated matched photocurrent. Interestingly, we reveal that this performance boost is achieved in perovskite films with thicknesses reduced by up to a 30% with respect to the standards, which not only facilitates charge carrier extraction but also reduces the use of material. This novel approach promises unprecedented perovskite-perovskite tandem efficiencies surpassing 30%, opening avenues for the realisation of next generation, affordable PV.

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Directional strong-coupling between nanolight and organic molecules

Ana I. F. Tresguerres-Mata[1†*]
O. G. Matveeva[2†], C. Lanza-García[1], K. V. Voronin[2], F. Calavalle[3], A. Tarazaga Martín-Luengo[1], J. Taboada-Gutiérrez[1,4], J. Duan[1,4], J. Martín-Sánchez[1,4], P. Díaz-Núñez[5], A. Bylinkin[2,3], R. Hillenbrand[3,6], A. Mishchenko[5], Luis E. Hueso[3,6], V. S. Volkov[7], A. Y. Nikitin[2,6*], P. Alonso-González[1,4*]

[1]*Department of Physics, University of Oviedo, Oviedo 33006, Spain*
[2]*Donostia International Physics Center (DIPC), Donostia/San Sebastián 20018, Spain*
[3]*CIC nanoGUNE BRTA, 20018 Donostia/San Sebastián, Spain*
[4]*Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo), El Entrego 33940, Spain*
[5]*Department of Physics and Astronomy, University of Manchester, Manchester, UK*
[6]*IKERBASQUE, Basque Foundation for Science, Bilbao 48013, Spain*
[7]*XPANCEO, Bayan Business Center, DIP, 607-0406, Dubai, UAE*

* anaiftresguerresmata@uniovi.es alexey@dipc.org pabloalonso@uniovi.es

Recent experiments have discovered the existence of low-loss nanolight – in the form of surface phonon polaritons (PhPs), i.e. infrared (IR) light coupled to lattice vibrations in polar crystals– with in-plane anisotropic (hyperbolic) propagation in the van der Waals (vdW) crystal α-MoO_3 [1]. Our results demonstrate that this exotic nanolight enables, for the first time, the visualization of directional-dependent strong coupling phenomena with organic molecules (pentacene). To support this claim, we will show near-field images taken by scattering-type scanning near-field optical microscopy (s-SNOM) on a curved flake of α-MoO_3 placed on top of a thin pentacene film (Figure 1), which allow us to directly corroborate the strong coupling variation as a function of the in-plane angle. This result opens the door to several new applications such as directional sensing or directional local control of chemical properties at the nanoscale.

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Figure 1

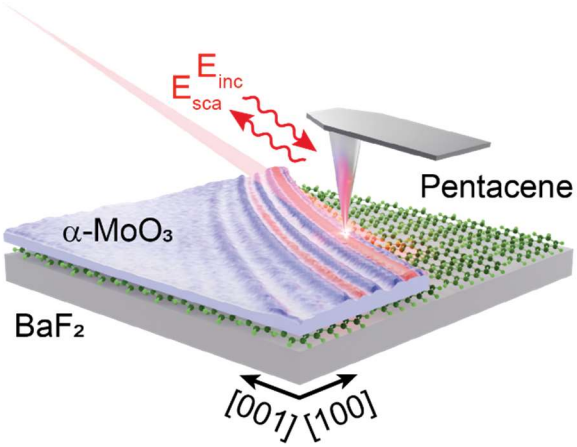

Figure 1: Schematic of the visualization by s-SNOM of strong coupling between PhPs and pentacene molecules.

Molecular electronics: insight from simulations and calculations

Andrés Martinez[1], Wynand Dednam[2], **Carlos Sabater[1]**
[1] *Departamento de Física Aplicada and Instituto Universitario de Materiales de Alicante (IUMA), Universidad de Alicante, Campus de San Vicente del Raspeig, E-03690 Alicante, Spain*
[2] *Department of Physics, Florida Science Campus, University of South Africa, Florida Park, Johannesburg 1710, South Africa*
carlos.sabater@ua.es

In the molecular electronics transport experiments performed via break-junction approach, it is challenging to identify the orientation of the molecule between the nanoelectrodes. To unmask the relationship between the orientation of the molecule and its conductance, we have combined atomistic simulations and ab *initio* calculations.
Our results obtained via classical molecular dynamics (CMD) using ReaxFF potential have shown the most typical orientations of the organic molecules when it is captured between the electrodes. Furthermore, for all the cases simulated we have calculated the electronic transport via Density Functional Theory (DFT) calculations. On the other hand, in our poster, we would like to present our friendly user interface for generating the inputs for DFT calculations and CMD simulations [ref. 2].

In order to test the validity of our model, we have compared our results with experimental measurements [ref. 1]. From this comparison, we can conclude that the model and the experiments are in good agreement.

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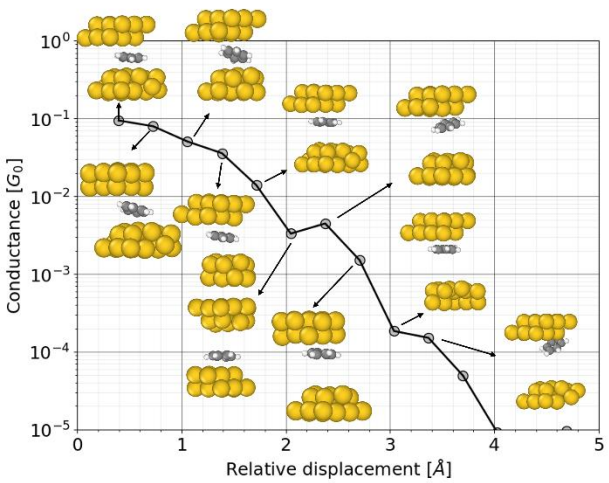

Figure 1: Electronic transport calculations versus relative displacement of the electrodes for the case of a single benzene molecule captured between gold electrodes. Inside we have illustrated the evolution of the contact simulated by CMD.

An apophatic description of spherical shells

Manuel Martín Bravo
Departamento de Ciencia, Computación y Tecnología, Universidad Europea de Madrid, 28670 Villaviciosa de Odón, Madrid, Spain.
manuel.martin@universidadeuropea.es

In semiconductor physics, a hole is a lack of an electron in the valence band of a semiconductor material. Holes are often referred to as positive charges, since the absence of an electron can be thought of as a "hole" that can be filled by an incoming electron, which would then be attracted to the positive charge.

Typical descriptions of shells such as spherical capsids are based on their actual building blocks like proteins. Recently, a more compact description in terms of absences of those units, which we may call holes, has been applied as well [1] and have proven to be a simpler way to predict icosahedral structures over spherical shells.

Holes play a significant role in the behavior of semiconductor materials and devices, such as transistors and solar cells. May holes become a useful concept in order to describe properties of shells other than simplifying their design process?

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Photocatalytic Janus microswimmers as microstirrers

Maximilian R. Bailey
Fabio Grillo, Lucio Isa
ETH Zürich, Vladimir-Prelog-Weg 1-5/10, Zürich, Switzerland
maximilian.bailey@mat.ethz.ch

Artificial microswimmers are micron-sized particles that convert energy sources such as light or chemicals into directed motion. Such "active" materials are thus intrinsically out-of-equilibrium, displaying emergent collective phenomena not observed in passive systems at thermodynamic equilibrium [1]. Active systems are promising for a range of autonomous applications, as they enable directed transport of matter at small scales, and can induce the mixing of fluids without external agitation [2]. Nevertheless, the mixing capabilities of increasingly dense suspensions of synthetic microswimmers have remained relatively unstudied to date. Here, we investigate the effect of microswimmer motion on the dynamics of passive tracer particles. Specifically, we increase the number density of our photocatalytic Janus microswimmers [3], and by simple scaling arguments, we demonstrate that enhancements in trace diffusivity predominantly occur via collisions with the microswimmers, similar to previous findings for living systems [4]. In doing so, we identify several limitations with the "chemistry-on-the-fly" microstirrers concept, as well as potential avenues to improve the overall mixing performance of synthetic active matter systems.

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Figures

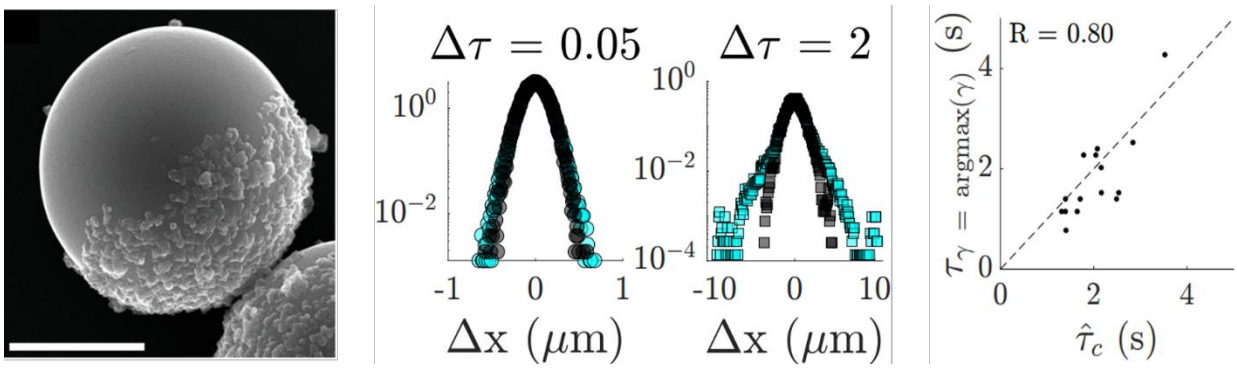

Figure 1: Influence of microswimmer motion on the dynamics of passive tracer particles. Left: HR-SEM of our synthesized, photocatalytic Janus microswimmers (scale bar 1 μm) (taken from [3]). Middle: Distribution of tracer displacements in the presence of microswimmers at different lag times ($\Delta\tau$ = 0.05s, 2s respectively) with (cyan) and without (black) tracer jumps extracted using the methodology provided in [4]. Right: Predicted collision time between microswimmers and passive tracers obtained from simple scaling arguments (x-axis) vs the experimentally observed lag time at which the kurtosis of the distribution of displacements (γ) is at its maximum (y-axis).

Graphene Liquid Gate Field Effect Transistors transducing amino acid fingerprints for protein sequencing.

César Pascual García1
Naveen Kumar2, Vihar Georgiev2
1 Materials Research Department, Luxembourg Institute of Science and Technology, Belval, Luxembourg;
*2 Device Modelling Group, James Watt School of Engineering, University of Glasgow, Glasgow, United Kingdom.*cesar.pascual@list.lu ; https://orcid.org/0000-0002-0526-2507

Protein sequencing techniques, which cannot provide detailed information for single point amino acids, are now limiting the use of proteins in the development of new personalized medicines. Important protein abnormalities in disease process, such as sequence alterations and aberrant post-translational modifications, are overlooked. In order to advance beyond the existing gold standard of mass spectrometry, new methods for distinguishing amino acid fingerprints must be developed. Amino acids are amphoteric proteins that adopt variable charge states based on the proton concentration in the surrounding environment (pH). They also have atomic interactions, which generate distinct molecular lengths and dielectric constants. These orthogonal properties can provide unique electrochemical signatures. Here, we calculate these fingerprints transduced by the surface potential and surface capacitance using standard models that include site-binding to account for proton affinity and the Stern-Gouy-Chapman theory to account for the interaction of charges in the electrolyte. To optimize the fingerprints, we investigate the impacts of the surface concentration of amino acids in the sensor and the ionic strength of the electrolyte. Our findings demonstrate the viability of measuring fingerprints for the 20 standard amino acids, which is not achievable by any of the other present or prospect approaches of protein sequencing currently under consideration. Finally, we highlight how graphene's features make graphene-liquid-gate-field-effect-transistors ideal sensors for detecting amino acid fingerprints.

Acknowledgement: This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 862539-Electromed-FET OPEN.

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Figures

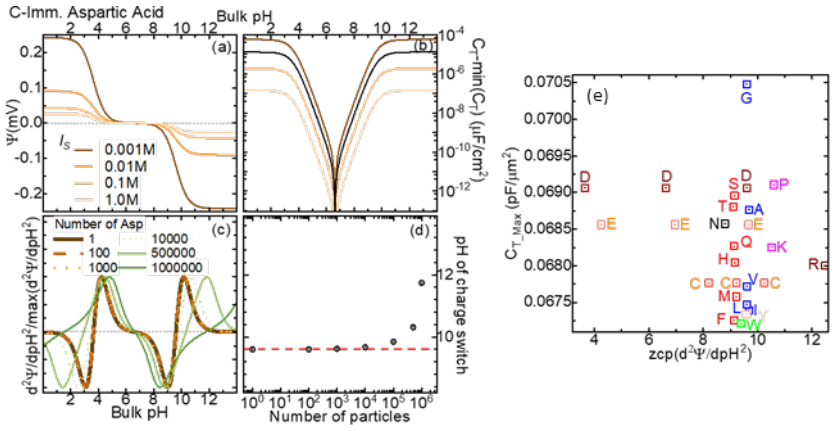

Figure 1: (a), (b)Surface potential (Ψ) and Capacitance (CT), respectively for 100 Aspartic acid molecules/μm2 at different Ionic strengths (IS). (c) d2Ψ/dpH2 at IS=0.01M for different numbers of molecules in 1μm2.(d) crossing of the alkaline switching charge, (red line indicates the nominal value of the pKb). (e) Calculations for fingerprints of 100 Amino Acids/ μm2 immobilized by the C-Terminal.

The uncanny weight of granular columns

R. Planet[1,2]
I. Zamorano, C. Anderson[1,3], and A. Fernandez-Nieves[1,2,3,4]
[1]*Department of Condensed Matter Physics, University of Barcelona, 08028 Barcelona, Spain;*
[2]*Institute for Complex Systems (UBICS), University of Barcelona, 08028 Barcelona, Spain;*
[3]*School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA;*
[4]*ICREA-Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain*
ramon.planet@fmc.ub.edu

Granular matter exhibits unusual mechanical properties. For example, when filling a cylindrical column with grains, the weight measured at the bottom of the column does not scale linearly with added mass, but asymptotically saturates towards a constant value. This observation is well-known in the granular matter community; it is referred to as the "Janssen's effect". The weight is partially supported by the lateral walls through frictional interactions with the grains. However, it has been recently observed that the weight measured at the bottom can become larger than the total added mass when the columns are sufficiently small compared to the diameter of the grains [1]. In this talk, we will review this "reverse" Janssen effect using grains with different geometries (spherical, oblate, and prolate particles). We find that all three geometries display the overshoot in weight, and we argue that packing effects are behind the quantitative differences between spherical to non-spherical grains. Finally, we will connect these results with recent experiments using fire ants as an active version of granular matter. Despite the inherent activity of the ants and their natural tendency to rearrange, the ants also develop force-chain structures that help support the weight of the column [2].

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FORC analysis in arrays of interacting nanodots

Alejandro Rivelles
M. Abuín, M. Maicas, J.L. Prieto and M.M. Sanz.
ISOM, Universidad Politécnica de Madrid, Madrid, Spain
Alejandro.rivelles.garcia@upm.es

FORC (first-order reversal curves) diagrams provide a lot of information about magnetic processes in a magnetic material by analyzing a large amount of minor hysteresis loops.
Interpretation of these diagrams is not straightforward, especially in complex systems with strongly interacting elements. Therefore, in many situations FORC diagrams are only used as magnetic signatures more than as a characterization technique. Recent developments in the method suggest that dividing the FORC plot in different regions, namely memory region and transient region, simplifies this analysis[1]. However, there is still a lack of understanding of the transient region, which reflects the magnetic vortex-like and multi domain particles behaviors in samples, that is essential for better understanding the method and could be applied to study novel magnetic textures, such as skyrmions or in areas like geomagnetism[2].
Nanodots are one of the simplest structures where vortex textures are presents. Therefore, and following a similar approach to previous works on nanostrips, in this work we analyze the interaction between Py and Co circular magnetic nanodots with different geometries, and compositions analyzing how the influence of magnetostatic interaction in the magnetic vortex texture is reflexed in the FORC distribution. Using magnetron sputtering and EBL lithography we have fabricated several samples with arrays of circular dots with a diameter of 200nm covering a total area of 3x3mm and varied the spacing between them thus modifying the magnetostatic interaction between elements. And regarding the composition we have fabricated samples with dots composed of two different magnetic layers separated by a non-magnetic layer and gradually separated them to analyze the effect of vertical magnetostatic interaction.
Finally, we have simulated with mumax3 FORC diagrams of arrays of nanodots varying the spacing between them, the size, and the height of the dots, obtaining similar results to the ones observed in the experimental measurements.

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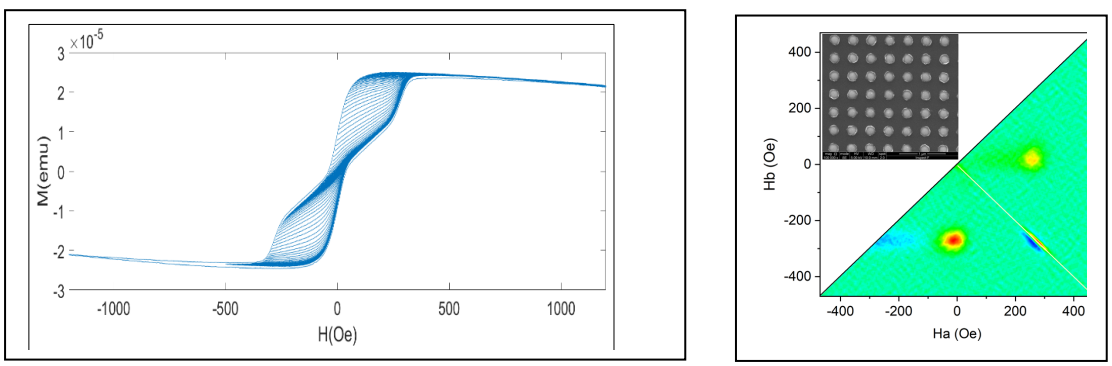

Figure 1: Example of the measurements for one of the samples, with non-interacting dots. On the right the FORC measurements taken with an AGFM, on the left the FORC distribution generated from the measurements and a SEM image of a portion of the array of nanodots.

Tunable magnetic equilibrium configurations in dipolar helices

Òscar Iglesias
Ot Garcés
Dpt. Física de la Matèria Condensada and IN²UB, Universitat de Barcelona, Av. Diagonal 645, 08028 Barcelona (Spain)
oscariglesias@ub.edu

The role that geometry and topology play in emergent order parameters has become an important topic in theoretical and experimental studies in different areas of physics [1]. A general theoretical framework to describe statics and dynamics of curved magnetic wires and surfaces has been developed recently, providing a starting point to study magnetization configurations in curvilinear structures [2]. New terms such as induced effective anisotropies and emergent Dzyaloshinskii-Moriya interactions appear because of curvature, which are responsible for magnetochiral effects, not present in the conventional cases. In this work, we have particularized the study to anti- and ferromagnetic (FM) helices, that are the simplest curves with constant κ and τ. By performing atomistic Monte Carlo simulations, we have validated the micromagnetic theoretical framework that predicts stable magnetization transitions between quasi-tangential (QT) to onion-like configurations [2]. Varying the curvature κ (or radius R) and torsion τ (or pitch p), we have obtained phase diagrams for the FM and AF cases for different kinds of magnetocrystalline anisotropies, extending them beyond the limits of application of the micromagnetic model. In a second part of the work, we will study the effects of curvature in systems where exchange determines the global magnetization direction, but the global magnetic order is dominated by dipolar interactions. This is the case of nanoparticle assemblies, colloidal magnets, magnetic beads or molecular clusters, that can be treated as magnetic macro-dipoles [3]. We will show that in dipolar helices a rich variety of equilibrium configurations can be reached by tuning the angle between consecutive dipoles. They include QT states, entwined head-to-tail magnetic helices that have a periodicity different from the generative helix and FM or AF ordered chains along the helix axis. Varying the radius or the pitch of the helix, abrupt transitions between states having zero and sizable net magnetization can be induced, which could be achieved experimentally by applying stress to the helix ends and be used as magneto-mechanic sensors. Work supported by Spanish MINECO (PID2021-127397NB-I00, PID2019-109514RJ-I00), DURSI (2017SGR0598) and EU FEDER funds (Una manera de hacer Europa) also CSUC for supercomputer facilities.

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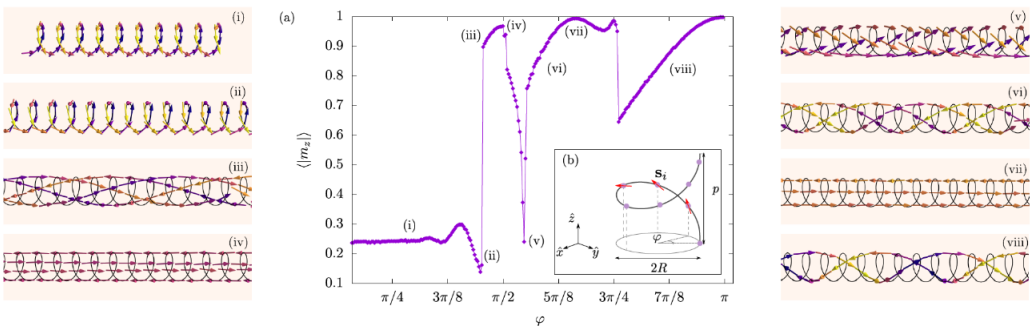

Figure: Ground states of a dipolar helix (R=1, p=π/2) and their staggered magnetization along the helix axis.

Strontium Titanium Chalcogenide Perovskite Photoanodes for H_2 Production

Jinan H. Al Shuhaib[1]
Nuria Jiménez-Arévalo[1], Elena Köhler[1], Fco. Javier García-García[2], José R. Ares[1], Isabel J. Ferrer[1,3], Fabrice Leardini[1,3]
[1]*Departamento de Física de Materiales, Universidad Autónoma de Madrid, Campus de Cantoblanco, E-28049 Madrid, Spain.*
[2] *ICTS-Centro Nacional de Microscopía Electrónica, Universidad Complutense de Madrid, E-28040, Madrid, Spain*
[3]*Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Campus de Cantoblanco, E-28049 Madrid, Spain*
jinan.awadh@estudiante.uam.es

Inorganic chalcogenide perovskites are semiconductors with general formula ABX_3, with A being a group II cation (i.e., Ca^{2+}, Sr^{2+}, or Ba^{2+}), B a group IV transition metal (i.e., Ti^{4+}, Zr^{4+}, or Hf^{4+}), and X a chalcogen anion (S^{2-} or Se^{2-}) [1]. These compounds present interesting optoelectronic properties, what make them of interest in different fields, such as energy harvesting. Some of these compounds have been poorly investigated to date. Here we present a novel synthesis procedure to obtain $Sr_{1+x}TiS_{3-y}$ powders. Moreover, we show for the first time an experimental characterization of some key properties of this compound, that may be relevant for many potential applications. First, we determine the crystalline structure by x-ray powder diffraction and electron diffraction. Tilting experiments of several crystals in the electron microscope tackled the reconstruction of the whole associated reciprocal lattice. In addition, high resolution electron microscopy images have been acquired for the first time in this compound. Next, we experimentally obtain its optical band gap (of about 0.96 eV) that corresponds to a direct allowed transition, in agreement with previous predictions.

Finally, we investigate the photo-electrocatalytic properties of these chalcogenide perovskites powders in a micro-electrolytic cell, by covering commercial screen-printed electrodes with our $Sr_{1+x}TiS_{3-y}$ powders (see Figure 1). We demonstrate that samples show good electrocatalytic activity and have significant photocurrents when used as photoanodes in Na_2SO_3 aqueous electrolytes. These results show that $Sr_{1+x}TiS_{3-y}$ has potential interest in hydrogen production by using renewable energy resources.

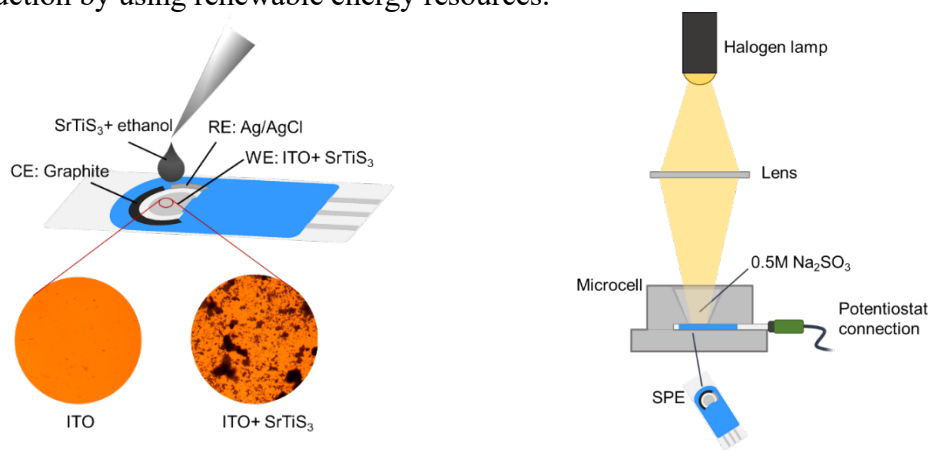

Figure 1. Schematic image of the drop coating method used to prepare the screen-printed electrodes (SPE) with our $Sr_{1+x}TiS_{3-y}$ powders and optical microscopy images of the prepared electrodes (left panel). Scheme of the micro-electrolytic cell used to determine the photo-electrolytic properties of the samples (right panel).

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Design and control of a Fresnel zone plate lens in silicon substrates

Maha Labani
Vito Clericò, Enrique Diez and Mario Amado
Nanotechnology Group, Departamento de Física Fundamental, Facultad de Ciencias University of Salamanca, Plaza de la Merced s/n 37008 Salamanca, Spain
idu018684@usal.es

X-ray microscopy has emerged as a technique to observe structures which are not accessible with conventional optical microscopy, and that has advantages in respect to electron microscopy due to the longer penetration depth and chemical sensitivity of the x-ray radiation. The optics of the x-ray microscopes includes components as the Fresnel zone plate lenses which are made by means of advanced nanofabrication techniques, such as high-resolution electron beam lithography. The period of the circular chirped grating that makes up the Fresnel zone plate decreases with increasing radius [1]. Both x-ray photons and other types of particles, like atoms [2] and neutrons [3] can be focused and imaged using these optical components. Here, we present the different steps of the Fresnel zone plate lenses fabrication. Since there is no mask required for electron beam lithography, we use the most simplistic approach through a CAD program to achieve a suitable design figure (1.a) that will be transferred onto a sacrificial Si substrate. In this work we will present a detailed study of the different processes involved in the generation of Fresnel Zone Plates (1.c) with special interest in the different etching processes with the aim to avoid a critical collapse of the desired structures.

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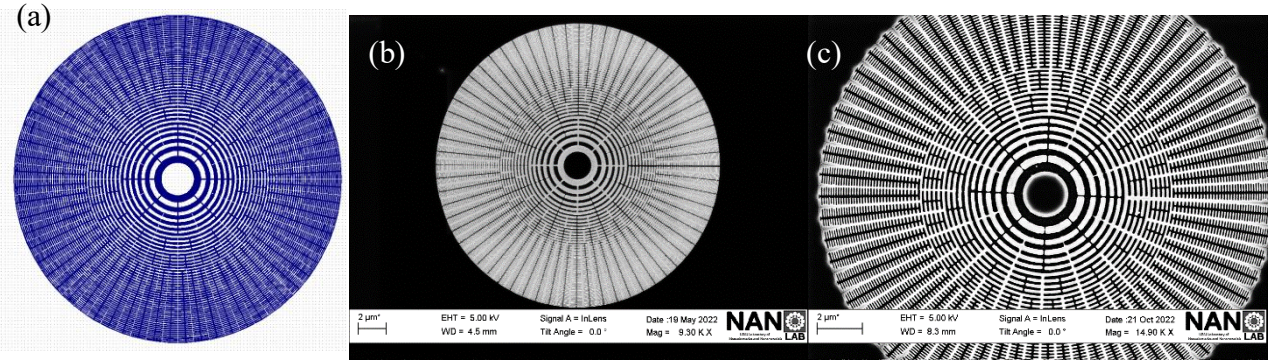

Figure 1: (a) CAD design of Fresnel zone lens, **(b)** Scanning electron microscope (SEM) image of FZP that has a diameter of 20 µm and an outermost zone width of 50 nm, **(c)** SEM overview of FZP after 15s of Silicone etching.

Plasmonic Rectification of terahertz radiation using encapsulated graphene field effect transistor

Abidi El Hadj[1]
J.A. Delgado-Notario[1], V. Clericó, J. Calvo-Gallego[1], J.E. Velázquez[1], C. Bray[2], C. Consejo[2], F. Teppe[2], T. Taniguchi[3], K. Watanabe[3], T. Otsuji[4] and Y.M. Meziani[1]
1/ Nanotech Group, Salamanca University, Facultad de Ciencias, Pza de la Merced, Ed. Trilingüe, Salamanca, Spain
2/ Laboratoire Charles Coulomb (L2C), UMR 5221 CNRS-Université de Montpellier, F-34095 Montpellier, France
3/ National Institute of Material Sciences, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan
4/ Research Institute of Electrical Communication, Tohoku University, Sendai 980-8577, Japan
elhadjabidi@usal.es

Plasmonic rectification of terahertz (THz) radiation is of great importance for the development of high-speed devices for THz technology [1,2]. Plasmonic rectifiers can be used to design efficient, sensitive, and compact devices that could operate at THz frequencies. In the present paper we report on THz rectification at 288 GHz by using an asymmetric dual grating field effect transistor based on an h-BN encapsulated graphene layer (Fig1-(a)). Photocurrent was measured at 1.7K at different top gate biases from 1 to -1V as shown in figure 1-(b) & (c). The first maximum was observed around the Dirac point as reported by other authors and a second one was observed around V_{BG}=1V at V_{TG}=0V. This peak has been tuned with the top gate to V_{BG}=8V for V_{TG}=-0.6V and to V_{BG}=-10V for V_{TG}=-1V. By biasing the metallic top and back gates, n and p type regions are created along the channel and above the gate fingers. The rectification of the incident THz light is interpreted as due to the plasmonic electron-hole ratchet mechanism in the graphene np junctions.

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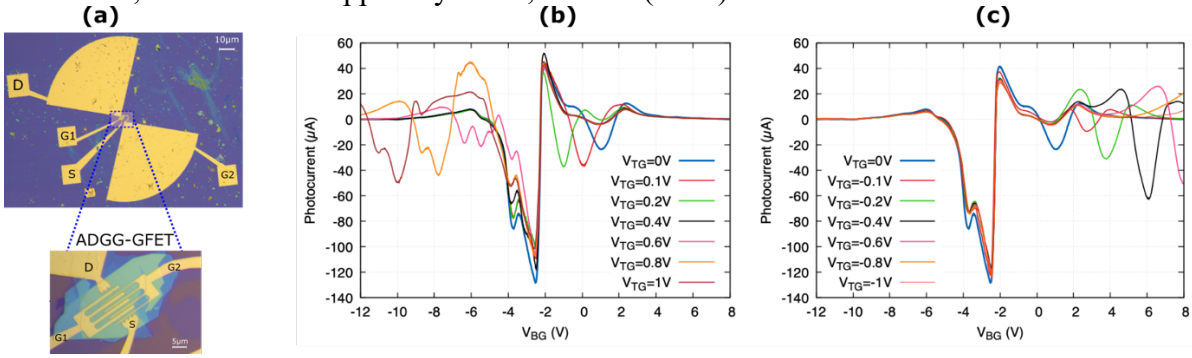

Figure 1: (a) Microscope photo of the ADGG-GFET and the measured photocurrent versus the back gate under excitation of 288GHz and at 1.7K for (b) positive top gates biases and (b) negative top gate bias

Acknowledgments

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Ga_2O_3:Cr nanowire-based optical microcavities for thermometry

Daniel Carrasco Madrigal[1]
Manuel Alonso-Orts[1], José M. San Juan[2], María Luisa Nó[2],
Alicia de Andrés[3], Emilio Nogales[1], and Bianchi Méndez[1]
1 Depto. Física de Materiales, Fac. CC Físicas, Universidad Complutense de Madrid, Madrid 28040, Spain
2 Depto. Física, Facultad de Ciencias y Tecnología, Universidad del País Vasco, Apdo. 644, Bilbao 48080, Spain
3 Inst. Ciencia Materiales de Madrid, CSIC, Cantoblanco, Madrid 28049, Spain
Email: daniecar@ucm.es

Gallium oxide is currently attracting great interest on the semiconductor field as it is a transparent conductive oxide (TCO) with an ultra-wide bandgap (~ 4.8 eV), high thermal and chemical stability and it can be doped with different ions such as Si, Sn, Cr^{3+}, Gd^{3+}, Er^{3+}, Eu^{3+} [1], making it a very suitable material for high power electronics and photonics applications [2]. A field of great interest for photonics applications are semiconductor micro- and nanowires whose optical properties can be controlled both by modifying the composition of the material and by creating artificial optical structures. A key photonic structure is the set of optical micro- and nanocavities based on distributed Bragg reflector (DBR), obtained by periodic modulations of the refractive index in a dielectric medium.
In this work, we present our recent results designing, optimizing, characterizing, and applying optical microcavities based on DBRs created within β-Ga_2O_3:Cr nanowires, which results in widely tunable Fabry-Perot (FP) resonances [3], and their use as wide dynamical range temperature sensors [4]. The analysis of their photonic behavior has been carried out both experimentally and with finite-different time-domain (FDTD) simulations. For the design of the thermometer, the thermal shift of two different PL features from the β-Ga_2O_3:Cr nanocavities is monitored: the characteristic R-lines of Cr^{3+} ions and the FP resonances. Combining both mechanisms, it can sense at least in the range of 150K to 550K with a precision around 1 K and a full width at half maximum of the FP peaks that is nearly unchanged in the whole temperature range.

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Figures

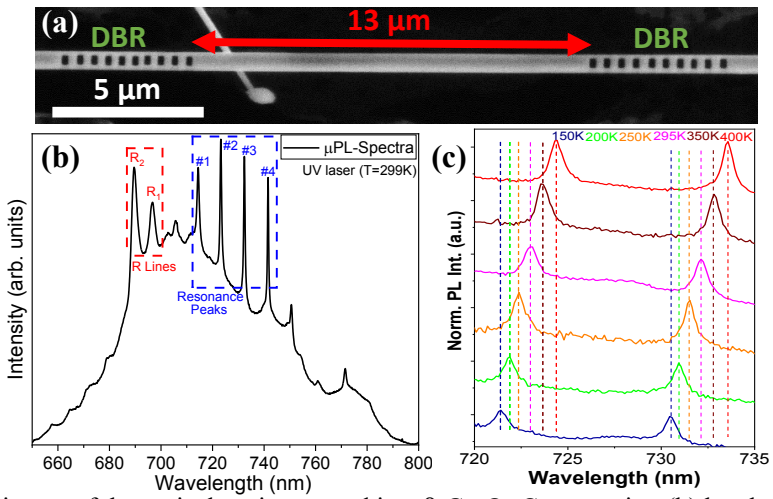

Figure 1: (a) SEM image of the optical cavity created in a β-Ga_2O_3:Cr nanowire, (b) local micro-photoluminescence spectrum for 299 K, (c) FP peak positions dependence on temperature.

Resonant tunneling energy harvesters: improving performance via quantum interference

José Balduque Picazo
Rafael Sánchez Rodrigo
Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
jose.balduque@uam.es

The spectral filtering of quantum dots can be used for heat to power conversion in electronic conductors. A proposal based on resonant-tunneling three-terminal devices [1] has been recently verified experimentally [2]. Two quantum dots connect the two terminals of a conductor to a hot electronic cavity where carriers exchange heat via thermalization. We propose the heat source to be separated from the conductor via a beam-splitter (e.g., the tip of a scanning microscope) that mediates the system-bath coupling. The resulting ballistic electron propagation gives rise to interferences [3] able to improve the engine performance, both in the extracted power and efficiency [4].

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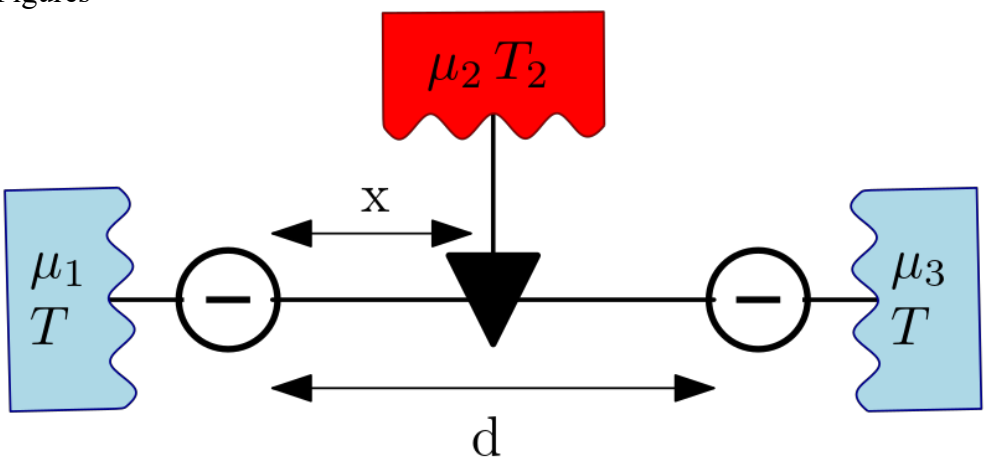

Figure 1: Sketch of the three-terminal device.

Exploiting nonlinearities of two-dimensional micro-drum resonators for random number generation

Ramón Bernardo Gavito[1], Julia García Pérez[1], and Daniel Granados[1]
[1] *IMDEA Nanociencia, Calle Faraday 9, Madrid, Spain*
ramon.bernardo@imdea.org

Random number generators are a key component in most cryptographic systems nowadays. In particular, true random number generators (TRNG) extract their entropy from an unpredictable physical processes that do not rely purely on mathematical algorithms. This reduces vulnerabilities from different types of attacks targeted to pseudo random number generators.

A widely used source of entropy for TRNG is the response of nonlinear oscillators [1], as they present bifurcations, chaotic behaviour and dynamical instabilities that render their response very difficult to predict even if their initial conditions are known.

Micro-drum resonators based on two-dimensional materials are a promising candidate to integrate as entropy source in cryptographic systems, as they present a strongly non-linear response and a high robustness [2].

In this work we explore different approaches to use few µm-wide electro-optical MoS_2 micro-drum resonators as randomness sources by applying frequency modulated signals close to their resonant frequencies in the range of tens of megahertz. Readout of the output is performed optically and the resulting signals present two distinct states, easing their interfacing with digital systems.

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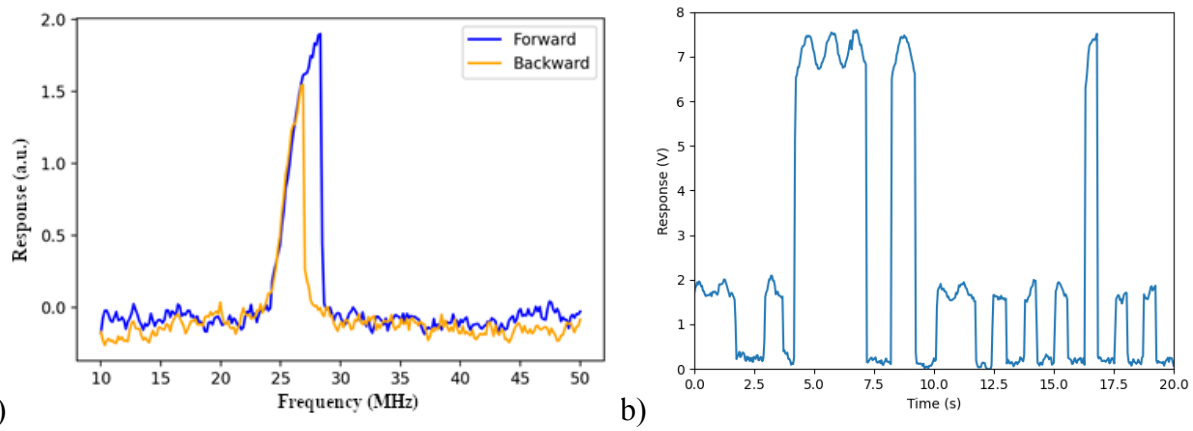

a) b)

Figure 1: a) Spectral response of one of our MoS_2 resonators showing a strong nonlinear behavior. b) Electrooptical response of the system under a slow-varying FM signal with a center frequency of 27.4 MHz and 500 kHz deviation.

Floquet theory of electronic stopping of nuclear projectiles in solids

Emilio Artacho,[1,2,3]
Marjan Famili,[3] Jessica F. K. Halliday,[3] Nicolò Forcellini[4]
[1] *CIC Nanogune BRTA and DIPC, Tolosa Hiribidea 76, 20018 San Sebastian, Spain*
[2] *Ikerbasque, Basque Foundation for Science, 48011 Bilbao, Spain*
[3] *Cavendish Laboratory, University of Cambridge, J. J. Thomson Ave., Cambridge CB3 0HE, United Kingdom*
[4] *Beijing Academy of Quantum Information Sciences, Beijing 100193, China*
e.artacho@nanogune.eu

Nuclei shooting through solids give rise to strongly non-equilibrium processes among electrons, which have been studied in different ways for decades due to their interest as prototypical quantum dynamical problems, but also due to their relevance to nuclear materials, space exploration and ion radiotherapy. We have been addressing the stationary states that arise when the projectile follows a periodic trajectory in a solid at constant velocity, by means of a Floquet theory of electronic stopping [1]. A first implementation in a tight-binding setting is used for illustration [2], as well as a characterisation of such stationary states for protons shooting across diamond in large-scale time-dependent density-functional theory calculations [3].

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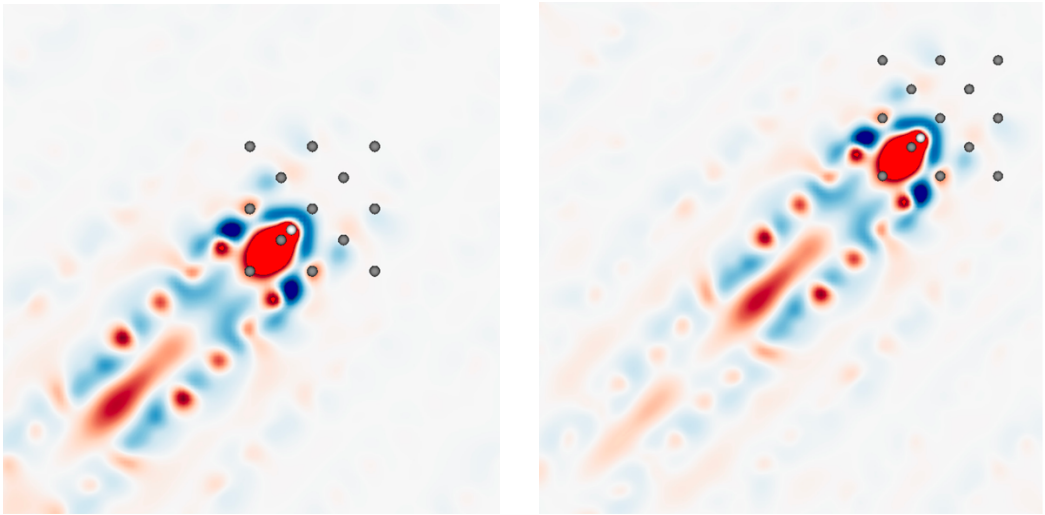

Figure 1: Electron deformation density in real space at equivalent projectile positions in consecutive diamond unit cells (left and right panels) along the trajectory for a proton moving at $v = 1$ a.u. along the [110] direction, depicted in the (001) plane containing the projectile. Color scale: from −0.01 e/Bohr (dark blue) to +0.01 e/Bohr (dark red), going through white for zero. Beads indicate atomic positions of selected atoms including the projectile (light bead) to indicate the equivalence of position under translation.

Pulsed plasmonic solid-state nanolasers assisted by 2D transition metal dichalcogenides

D. Hernández-Pinilla[1]
P. Molina[1], G. López-Polín[1], J. H. Al Shuhaib[1], F. Leardini[1], H. Yan[2], Y. Wang[2], S. Sarkar[2], M. Chhowalla[2], P. Ares[3,4], J. Gómez[3,4], M. O Ramírez[1,4], L. E. Bausá[1,4]
[1]*Dept. Física de Materiales, Universidad Autónoma de Madrid, Madrid, Spain*
[2]*Dept. of Materials Science & Metallurgy, University of Cambridge, Cambridge, UK*
[3]*Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain*
[4]*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain*

david.hernandezp@uam.es

The combination of optical gain media with plasmonic nanostructures has allowed the emergence of nanolasers with subwavelength confined modes. However, with the exception of a scarce number of systems[1], which in addition are limited by cryogenic operation and thermal stability, lasing in the subwavelength scale occurs exclusively in continuous wave regime. In this context, the realization of pulsed nanolasers based on solid-state gain media represents a relevant boost to deal with the variety of near and far field applications that require the intrinsic advantages of solid-state lasers, such as high thermal and chemical stability.[2,3]

Here, we associate two-dimensional (2D) transition metal dichalcogenide (TMD) with a plasmon-assisted solid state nanolaser to simultaneously enable temporal and spatial confinement of the laser gain in a monolithic architecture (Fig 1). The hybrid system combines a Nd^{3+} doped solid-state crystal which provides laser gain in the NIR spectral region, plasmonic chains of Ag nanoparticles that enables subwavelength spatial confinement of laser radiation, and a 2D TMD acting as saturable absorber to achieve the temporal confinement of laser radiation by means of passive Q-switch. Different configurations are analyzed. In particular, stable laser pulse trains in the ns and μs temporal domains have been successfully obtained at the nanoscale with subwavelength confinement at room temperature. The results show the potential of pulsed solid-state nanolasers to face the challenges in many applications such as photolithography for ultra-small motif size fabrication, ultra-compact integrated circuits or biodetection, with the added value of reduced energy consumption.

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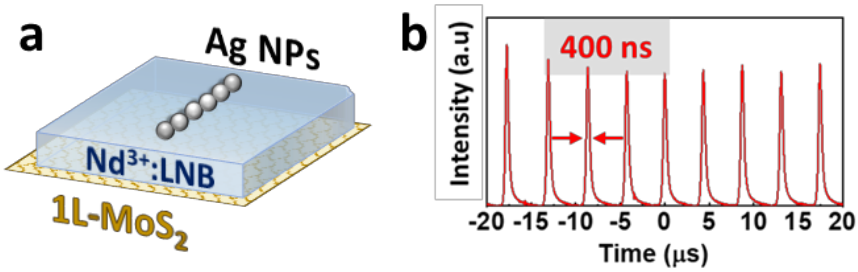

Figure 1: a) Schematics of the monolithic architecture for pulsed nanolasing. The hybrid system includes: Nd^{3+}-doped $LiNbO_3$ as a gain media, plasmonic Ag nanoparticle chains for sub-wavelength spatial confinement, and 1-layer MoS_2 for temporal confinement of laser radiation. b) Temporal evolution of laser emission.

Scalable and low-cost fabrication of flexible WS_2 photodetectors on polycarbonate.

Jorge Quereda
Co-Authors (Font size 10)
Sruthi Kuriakose, Carmen Munuera, Federico J Mompean, Abdullah M Al-Enizi, Ayman Nafady, Enrique Diez, Riccardo Frisenda, Andres Castellanos-Gomez
Email: jorquere@ucm.es

We present a low-cost and easy-to-implement technique to fabricate large-area WS_2 photodetector devices onto transparent and flexible polycarbonate substrates. The method relies on the deposition of large-area (in the cm scale) thin films (~30 nm thick) of WS_2 by a recently introduced abrasion-induced method. Interdigitated electrical contacts are then deposited by thermal evaporation through a shadow mask. The photodetectors present well-balanced performances with an good trade-off between responsivity (up to 144 mA/W at a source-drain voltage of 10 V and illumination power of 1 μW) and response time (down to ~70 μs) and a detectivity value of 10^8 Jones. We found that the devices perform very reversibly upon several illumination and straining cycles and we found a moderate device-to-device variation.

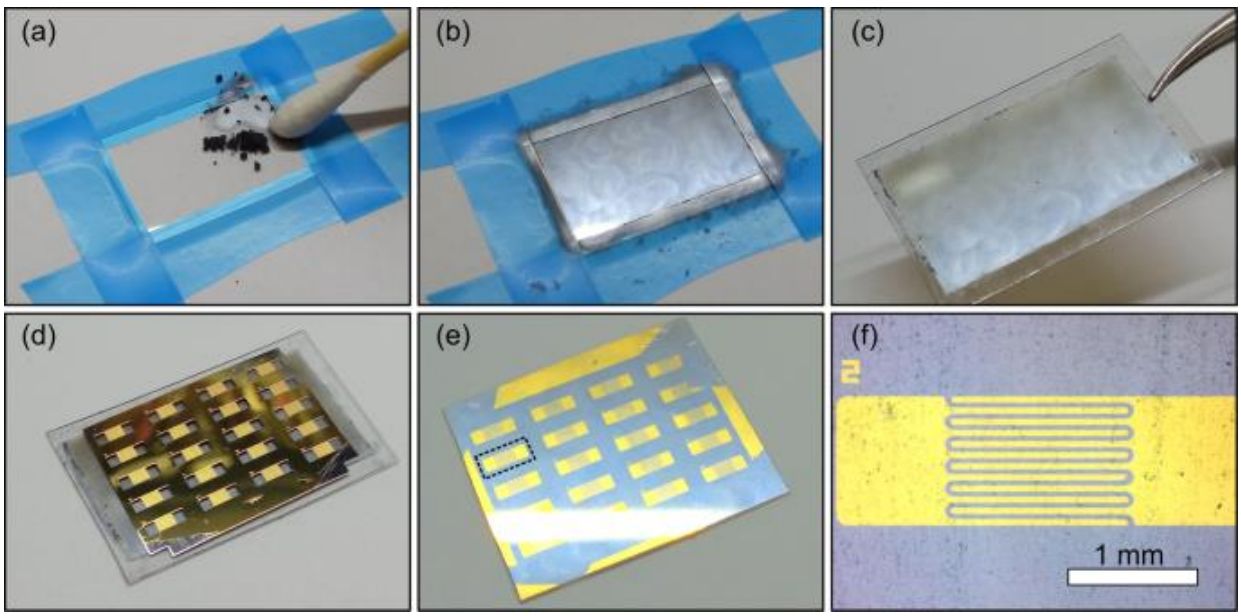

Figure: a Fine WS_2 powder is rubbed against the surface of a polycarbonate substrate with a cotton swab. **b, c** Pictures of the WS_2 film on polycarbonate after deposition. **d** A shadow mask is placed onto the surface of the film. **e** Picture of a polycarbonate chip after the evaporation of 20 devices. **f** Higher magnification image of one of the devices, highlighted with a dashed rectangle in e.

Photoluminescence properties of carbon nanodots with high nitrogen level

Rania Doudi[1]
José Antonio Novoa[2], Íñigo J. Sola[2], Chahinez Berrah[2], M. Dolores Merchán[1] and M. Mercedes Velázquez[1]
[1] Nanotechnology group, Department of Physical Chemistry, University of Salamanca, Spain. [2] Laser applications and photonics ALF group, Department of Applied Physics, University of Salamanca, Spain
zigi.rania@gmail.com

Carbon nanodots, CNDs, constitute a vast family of carbonaceous materials synthesized by different procedures with diameters above 10 nm. They present different chemical composition, size, and photoluminescence (PL) properties depending on the route used for synthesis. Their unique properties, strong fluorescence, tunable band gap, low toxicity and cost, and high-water solubility have led to numerous applications, such as catalysts, optoelectronic devices, biosensors, and solar cells. It is well established that the PL emission of carbon dots consists in a band (blue PL) corresponding to the energy transition of the carbon core ($\pi \rightarrow \pi^*$). However, in some applications, especially in biology, that emission presents important limits due the background of some biomolecules. Therefore, the synthesis of carbon nanodots with long wavelength emissions is necessary. To modulate the PL emission of carbon nanodots, doping with electron-deficient or electron-rich atoms have been suggested. Nitrogen is one of the most widely used dopant since doping procedures are relatively easy and N-doped CNDs present excellent photoluminescence properties. However, the origin of the photoluminescence is poorly understood. Therefore, to clarify the origin of the PL in N-doped CNDs, we analyzed the effect of the chemical composition on the photochemical properties of N-doped CNDs. To synthesize materials with different N-doping we selected the hydrothermal treatment at 150º C during 8h using citric acid (CA) and distilled ethylene diamine (ED) as carbon and nitrogen precursors and changing the ED/CA ratio between 1 and 3. After that, the solution was filtered and dialyzed for 2 days to remove all unreacted impurities. Through this procedure, we obtained CNDs with high N-doping degree (15-18%). The size of the N-doped CNDs was determined by DLS and TEM and increase from 15.8 to 29 nm as the percentage of N. XPS measurements show the existence of 3 different C-N bonds, pyridinic, pyrrolic and graphitic. The percentage of each bond changes with the N content. From the XRD diffractograms, the interlayer distance, d_{002}, was determined and related with the pyrrolic bonds. Samples in time-resolved fluorescence measurements were excited by means of the combination of a femtosecond CPA laser (pulse duration: 60 fs) and an optical parametric amplifier (OPA). Thus, the central wavelength of the excitation ultrafast pulses could be tuned from 235 nm to 2400 nm. The fluorescence was time-resolved by means of a spectrograph with a gated intensified camera. From the analysis of absorption, emission, excitation spectra and the fluorescence decays, we conclude that the fluorescence emission is due to four emissive centers assigned to $\pi \rightarrow \pi^*$ transition for aromatic domains in zigzag and armchair configurations, charge-transfer, and $n \rightarrow \pi^*$ transitions. We also report correlations between the charge-transfer emission and the percentage of pyrrolic and pyridinic N-groups and between the $n \rightarrow \pi^*$emissions and the pyridinic bonds. Furthermore, we show that the charge-transfer emission is quenched by the carbonyl groups at the basal plane of the nanoparticles.

Multipole description of optical spatial dispersion in crystals

Óscar Pozo Ocaña
Stepan S. Tsirkin and Ivo Souza
Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain
oscar.pozo@ehu.eus

Natural optical activity is the paradigmatic example of an effect originating in the weak spatial inhomogeneity of the electromagnetic field on the atomic scale. Such effects are well described in molecules by the multipole theory of electromagnetism, where the coupling of light is treated semiclassically beyond the electric-dipole approximation. That theory has two shortcomings: it is limited to bounded systems, and its building blocks - the multipole transition moments - are origin dependent. In this work, we recast the multipole theory in a translationally-invariant form that remains valid for periodic crystals. Working in the independent-particle approximation, we introduce "intrinsic" multipole transition moments that are origin independent and transform covariantly under gauge transformations of the Bloch eigenstates. Electric-dipole transitions are given by the interband Berry connection, while magnetic-dipole and electric-quadrupole transitions are described by matrix generalizations of the intrinsic magnetic moment and quantum metric. In addition to multipolar terms, the response of crystals at first order in the wavevector of light contains band-dispersion terms that have no counterpart in molecular theories. The rotatory-strength sum rule for crystals is found to be equivalent to the topological constraint for a vanishing chiral magnetic effect in equilibrium, and the formalism is validated by numerical calculations on a tight-binding model of a chiral crystal.

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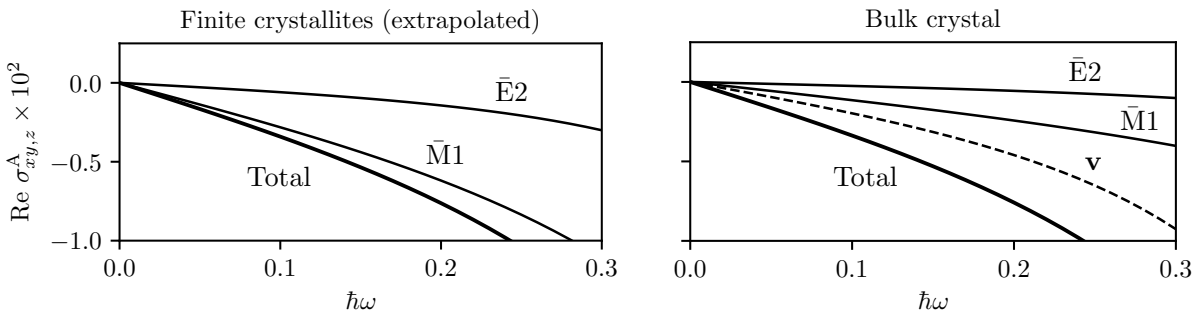

Figure 1: Decomposition of the spatially-dispersive conductivity tensor into three types of origin-independent contributions: intrinsic magnetic dipole (M1), intrinsic electric-quadrupole (E2) and band-dispersion (v). The latter is only present in the bulk calculations on the right, and it must be included to obtain the same total result as in the extrapolated crystallite calculations on the left.

Fabrication of Single Photon Emitters in Hexagonal Boron Nitride by Ion Irradiation

Julia García Prieto[1]
Abel Martínez-Suárez[1,2], Adam Roselló[1,3], Dimas Oteyza[2,3], Aitana Tarazaga Martín-Luengo[1], José Olivares[4,5], Pablo Díaz[4,5], Pablo Alonso-González[1,2], Javier Martín-Sánchez[1,2]
[1]*Departamento de Física, Universidad de Oviedo, Oviedo, Spain*
[2]*Nanomaterials and Nanotechnology Research Center (CINN-CSIC), El Entrego, Spain*
[3]*Donostia International Physics Center (DIPC), Donostia/San Sebastián, Spain*
[4]*Instituto de Óptica "Daza de Valdés" CSIC, Madrid, Spain*
[5]*Centro de Microanálisis de Materiales CMAM-UAM, Madrid, Spain*
uo243498@uniovi.es

The development of novel ultra-compact two-dimensional (2D) photonic technologies for application in quantum information processing, relies on our ability to fabricate single photon sources in 2D van der Waals materials with control of their optical emission properties, and preferably working at room temperature (RT). Recently, the possibility of obtaining single photon emission from 2D hexagonal boron nitride (h-BN) crystals at RT has been demonstrated, attributed to the presence of defects states within its wide bandgap [1], which has triggered an intense research activity in the last years [2]. In this regard, the deterministic fabrication of such emitters in h-BN has been tackled by different techniques such as thermal annealing [3], plasma treatment [4] or electron irradiation [5].

In this work, we present a systematic study by employing ion irradiation for different fluence and kinetic energy values. Specifically, a set of samples consisting of 2D h-BN flakes obtained by mechanical exfoliation has been irradiated using a variety of light (H) and heavy (Si, C, Cl) ions. We clearly observe formation of quantum emitters in the irradiated flakes in comparison with pristine flakes where a relatively low density of emitters is measured. The emission energy and emitters density in irradiated h-BN 2D crystals is discussed based on micro-photoluminescence time-resolved and time-correlated characterizations.

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Analysis of femtosecond-laser induced damage tracks in non-linear crystals by second-harmonic-generation microscopy

Ignacio López Quintás
Nuria Sevilla Sierra, Mª Jesús Martínez Morillo, Javier R. Vázquez de Aldana
Grupo de Investigación en Aplicaciones del Láser y Fotónica, Universidad de Salamanca, Pl. La Merced SN. 37008 Salamanca, Spain.
ilopezquintas@usal.es

Non-linear microscopy (including second-harmonic and third-harmonic generation as well as two-photon fluorescence) is a family of advanced laser-scanning microscopy techniques in which confocal operation appears in an intrinsic way [1]. It has been successfully used in different fields, such as biology, medicine or material science. On the other hand, femtosecond laser pulses have become an excellent tool for the 3D nano/micro-structuring of transparent solids. The high intensity reached in the focal region of a focused femtosecond pulse produces a non-linear ionization of the target that leads to a permanent and controllable local modification (i.e., refractive index change). Based on this modification, integrated photonic devices can be fabricated [2].
In this work we present our results of second-harmonic microscopy (SHM) for the analysis of femtosecond laser induced damage tracks in a BaB_2O_4 (BBO) crystal, which is a paradigmatic material for non-linear applications. SHM has been previously employed for the analysis of photonic devices (waveguides) in non-linear crystals [3] but, to our knowledge, no detailed study of the effect of the laser irradiation on the target non-linear properties has been reported.

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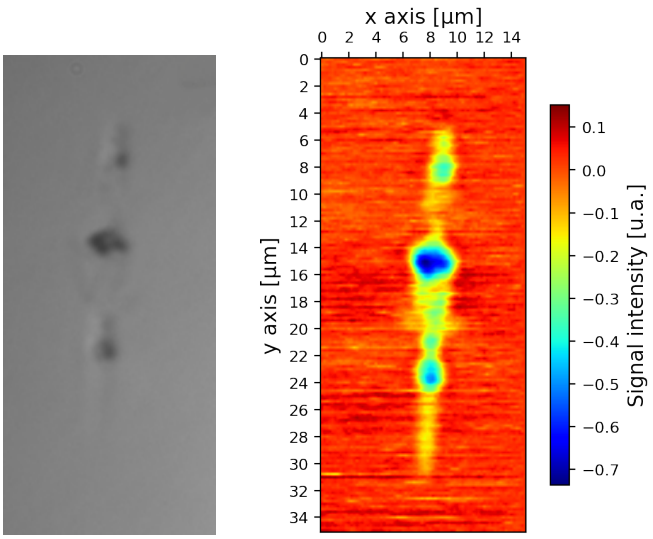

Figure 1: Example of the obtained results. Left; Optical image of a damage track induced at 118 µm below the surface of a BBO crystal with 60 fs, 60 mW pulses. Right; Corresponding SHM map of the damage track.

Emergence of Floquet band structure in Dirac Hamiltonians by short pulse irradiation

Yuriko Baba[1,2]
Vanessa Junk[2], Francisco Dominguez-Adame[1], Rafael A. Molina[3], Klaus Richter[2]
[1]*Departamento de Física de Materiales, Universidad Complutense de Madrid, Madrid, Spain*
[2]*Fakultät für Physik, Universität Regensburg, Germany*
[3]*Instituto de Estructura de la Materia, IEM-CSIC, Madrid, Spain*
yuribaba@ucm.es

Floquet theory is a well-established approach to describe time-dependent quantum systems driven by a periodic external field. In the presence of such a driving, the spectrum of the system is described by replicas of the original dispersion, shifted by integers of the driving frequency. Nevertheless, in most experiments with strong driving fields, the external field is applied in a short pulse lasting only a few periods. Using the Floquet formalism, this work studies from a theoretical perspective the emergence of the Floquet structure in the energy spectrum of Dirac Hamiltonians [1] subject to short pulses in order to understand the limits of this formalism as well as to interpret recent results of subcycle lightwave-ARPES [2].

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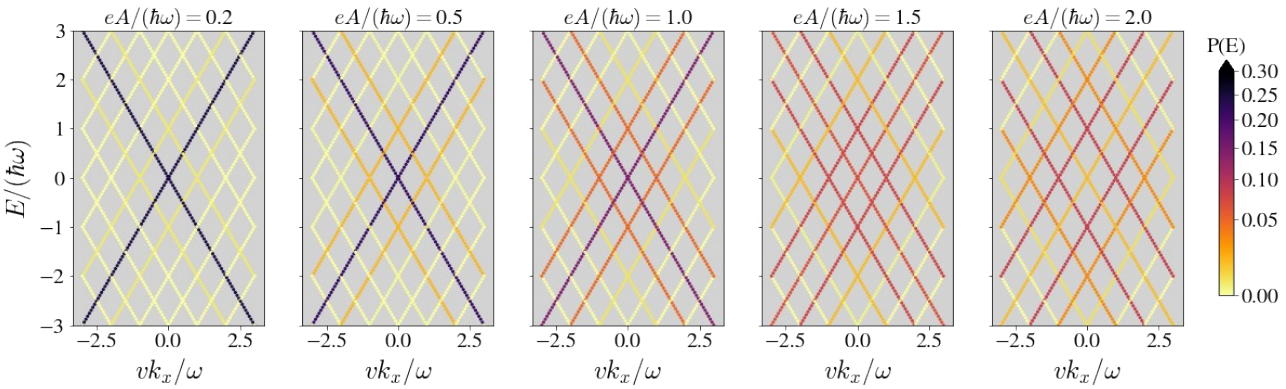

Figure 1: Spectral density projected onto the Floquet replicas for a Dirac Hamiltonian and a linearly polarized driving.

Twistoptics: Anisotropic Polaritons in Heterostructures made of an Arbitrary Number of Rotated Thin Layers

José Álvarez-Cuervo[1,2]
Christian Lanza[1,2], Aitana Tarazaga Martín-Luengo[1,2], Gonzalo Álvarez-Pérez[1,2], Kirill V. Voronin[4], Nathaniel Capote-Robayna[4], Javier Martín-Sánchez[1,2], Alexey Y. Nikitin[3,4] and Pablo Alonso-González[1,2]

1. *Department of Physics, University of Oviedo, Oviedo 33006, Spain.*
2. *Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo), El Entrego 33940, Spain.*
3. *Donostia International Physics Center (DIPC), Donostia-San Sebastián 20018, Spain.*
4. *IKERBASQUE, Basque Foundation for Science, Bilbao 48013, Spain.*

Email: uo257242@uniovi.es

Polaritons in strongly anisotropic media have recently emerged as a promising tool for controlling light at the nanoscale. Among them, understanding phonon polaritons (PhPs) in biaxial van der Waals crystals [1] arise as one of the cornerstones for future communication and sensing devices at the mesoscopic regime. In this sense, twisted heterostructures made of biaxial slabs offer singular properties, such as strong confinement [2], canalization, ultralow losses and topological transitions [3], among others. However, a general theoretical model that describes the light propagation in these systems is still needed. Here, a complete general derivation of a model for a system made of an arbitrary number of rotated biaxial slabs is performed. An extension to simpler systems made of anisotropic materials and a comparison with their analytical models is also detailed in this paper, showing a perfect agreement with previous models [4,5]. All calculations are compared with full-wave electromagnetic simulations. This work lays the foundations for future experiments in the field of twistoptics, allowing for a theoretical prediction and justification of the behavior of electromagnetic modes in heterostructures made of twisted biaxial slabs measured by near-field techniques.

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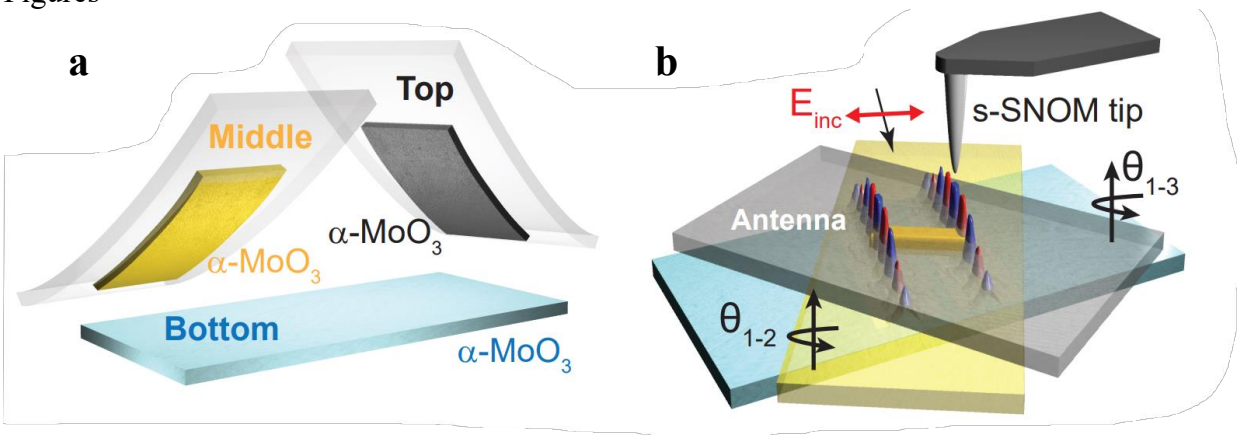

Figure 1: (**a**) Schematic of a twisted biaxial system made of three α-MoO3 layers. (**b**) Schematic of the excitation of polaritons in a twisted biaxial system by a scattering-type scanning near-field optical microscopy (s-SNOM).

Supression of superradiance by magnetic correlations

Sebastián Roca Jerat
Marcos Rubín
David Zueco
Fernando Luis
Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC – Universidad de Zaragoza, Zaragoza, 50009, Spain
sroca@unizar.es

One of the most exciting footprints of quantum physics lies in the collective behavior exhibited by many body systems. The correlations between atoms in an ensemble give rise to phenomena far richer than the sum of individual behaviors could ever be. One of these is superradiance [1], the interaction between light and matter generates long-range correlations that result in collective atomic states which (super)radiate. Another origin of such correlations can be the interaction between the atoms of the ensemble themselves [2]. Although both interactions play a fundamental role in many fields, especially light-matter in quantum computation [3], the competition that may arise between them in the same system seems to be rather unexploited. Here, we study the interaction of microwave radiation propagating via a superconducting co-planar transmission waveguide with model spin-1/2 DPPH molecules [4] whose magnetic correlations are controlled by modulating either the external magnetic field ($0 < \mu_0 H < 1$ T) or temperature (10 mK < T < 4.2 K). It is found that, above 1K, the system is in a uncorrelated paramagnetic phase and the emission is superradiant. However, below this temperature, an anisotropic magnetic interaction onsets correlations between the molecules building one-dimensional chains that suppress superradiance [Cf. Figure 1]. These results allow exploring new states of matter, arising from the interplay between magnetic and light-matter couplings, and provide a tool to externally control superradiance.

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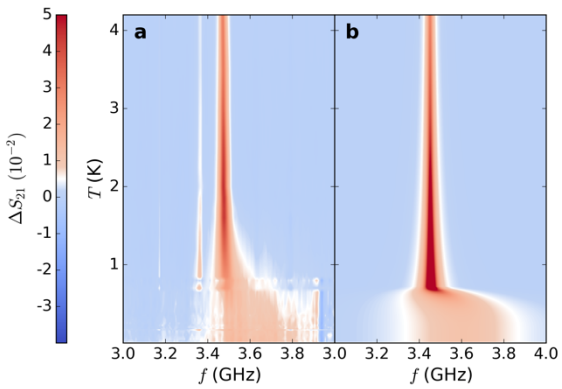

Figure 1: Supression of superradiance as low temperatures onset magnetic correlations. (a) Experimental transmission and its theoretical simulation (b).

Silver nanoparticle chains as subwavelength guides for ultra-long-distance fluorescence transmission

Javier Fernández-Martínez[1*],
Sol Carretero-Palacios[1], Pablo Molina[1], Jorge Bravo-Abad[2], Mariola O Ramírez[1] and Luisa E. Bausá[1]
[1]*Dept. de Física de Materiales, Instituto de Ciencia de Materiales Nicolás Cabrera (INC) and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049-Madrid, Spain*
[2]*Dept. de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049-Madrid, Spain*
[*]javier.fernandezm@uam.es

The manipulation and control of the emission properties of Rare Earth (RE) ions is currently a field of intense research due to the applicability of these emitters in a variety of technological fields such as sensing, green energy, bioimaging or quantum technologies [1]. In this context, the association of plasmonic nanostructures with RE-doped crystals has been revealed as an interesting approach, offering solid-state platforms with emergent functionalities at subwavelength scales. Among others, dual wavelength laser operation enabled by plasmonic structures in RE-doped crystals and plasmon-induced spatial coherence in RE emitters have been recently demonstrated [2,3].
In this work, the association of plasmonic arrangements with RE ions is further exploited to demonstrate the possibility of guiding the fluorescence of Nd^{3+} ions at ultra-long distances in the sub-wavelength regime by means of plasmonic chains of silver nanoparticles (NPs). Such plasmonic nanostructures exhibit an intense and spectrally broad longitudinal mode, which extends from the VIS to the NIR region, overlapping most of the spectral regions in which Nd^{3+} transitions occur [4].
The fluorescence guiding along the silver chains is monitored by means of dual confocal fluorescence microscopy that enables the spatial separation of the excitation and emission beams. The possibility of sub-wavelength fluorescence propagation is demonstrated over tens of microns in the NIR spectral region in which Nd^{3+} ions emit.
The results are explained considering the near field coupling of the Nd^{3+} emitting ions with the collective plasmon modes of the Ag NP chains, given the low dissipative losses displayed by the collective longitudinal mode supported by the closely spaced interacting NPs in the plasmonic chain. Numerical simulations based on the finite-difference time-domain method were used to analyze the response of the plasmonic chain when excited by an oscillating dipole representing the Nd^{3+} ion. The obtained results revealed the formation of strong hotspots extending up to 5 microns beyond the point dipole, in good agreement with the experiments.
The work evidences the potential of plasmonic nanoparticle chains as ultralong-range waveguides with extreme light confinement and proves their applicability in integrated hybrid plasmonic-photonic circuits in the technologically interesting NIR region.

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Unconventional fermions and where to find them: linear and nonlinear optical responses of multifold semimetals CoSi and RhSi

Miguel Ángel Sánchez Martínez[1,2]
Bing Xu[3], Zhenyao Fang[4], Zhuoliang Ni[4], Baozhu Lu[5], S. Sayyad[1,6], Jörn W. Venderbos[4,7], Fernando de Juan[1,8], Liang Wu[4], Darius H. Torchinsky[9], Adolfo G. Grushin[2]
[1]*Donostia International Physics Center, P. Manuel de Lardizabal 4, 20018 Donostia-San Sebastian, Spain*
[2]*Institut Néel, CNRS and Univ. Grenoble Alpes, 38042 Grenoble, France*
[3]*University of Fribourg, Department of Physics and Fribourg Center for Nanomaterials, Chemin du Musée 3, CH1700 Fribourg, Switzerland*
[4]*Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, 19104 Pennsylvania, USA*
[5]*Department of Physics, Temple University, Philadelphia, PA 19122, USA*
[6] *Max Planck Institute for the Science of Light, Erlangen, Germany*
[7]*Department of Physics, Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennsylvania 19104, USA*
[8]*IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain*
[9]*Department of Physics, Temple University, Philadelphia, PA 19122, USA*
miguelangel.sanchez@dipc.org

The 230 space groups, of which only 65 are chiral, describe all possible combinations of non-magnetic crystal symmetries in nature. Materials described by some of these groups host band degeneracies near the Fermi level protected by the corresponding crystal symmetries. A remarkable example of materials exhibiting this type of degeneracies are the topological semimetals RhSi and CoSi. The low-energy quasiparticles emerging near the protected band degeneracies, referred to as multifold fermions, have no counterpart as elementary fermionic particles. We present in this talk the linear optical conductivity of all chiral multifold fermions[1] and show that it provides an experimental fingerprint for each type of multifold fermion. We use a tight-binding model for space group 198, where RhSi and CoSi crystallize, revealing that the location of the chemical potential is crucial to understand the optical response seen in experiments[2,3], determined at low energies by the threefold fermion at the Γ point in both materials, and providing signatures of the existence of a spin-3/2 fourfold fermion in CoSi. Finally, we study the second-harmonic generation of RhSi. We analyze the experimental results using a second-order k·p Hamiltonian and compare our results with density functional theory calculations to provide a comprehensive description of the origin of the different features in the second-harmonic response and their relation to the topological character of the bands in RhSi.

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*Equally contributing authors

Quantum chaos in the Bose-Hubbard model

Alberto Rodríguez[1]
Lukas Pausch[2], Edoardo G. Carnio[3], Andreas Buchleitner[3]
[1]Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain
[2]CESAM Research Unit, University of Liège, 4000 Liège, Belgium
[3]Physikalisches Institut & EUCOR Centre for Quantum Science and Quantum Computing, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, 79104, Freiburg, Germany
argon@usal.es

We identify the chaotic phase of the Bose-Hubbard Hamiltonian by the energy-resolved correlation between spectral features and structural changes of the associated eigenstates as exposed by their generalized fractal dimensions (Fig. 1). The eigenvectors are shown to become ergodic in the thermodynamic limit, in the configuration space Fock basis, and we demonstrate that the fluctuation of the generalized fractal dimensions among near-in-energy eigenstates is a rather sensitive probe of quantum chaos with a qualitative basis-independent behaviour [1,2].

We scrutinize the chaotic phase of the model as function of particle number and system size in relation to several random matrix ensembles, and find that, as the limit of infinite Hilbert space is approached, the fastest route to chaos is the path at fixed particle density $n \leqslant 1$ [3]. While random matrix theory (RMT) gives a good description of coarse-grained spectral and eigenvector features in the chaotic phase, we show that, in terms of the fractal dimension distribution, the Bose-Hubbard model departs from RMT as Hilbert space grows [1-3]. These results provide further evidence of a way to discriminate among different many-body Hamiltonians in the chaotic regime.

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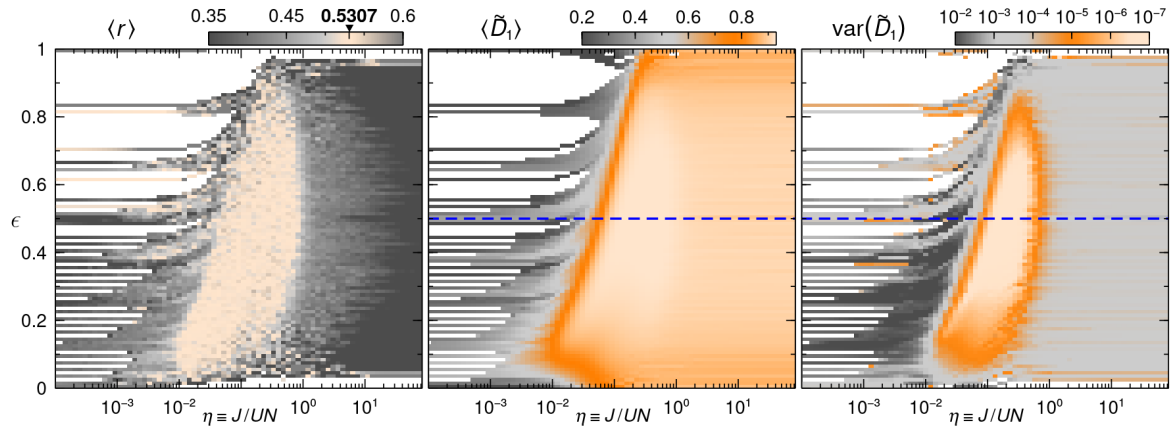

Figure 1: Chaotic phase of the Bose-Hubbard Hamiltonian exposed by spectral statistics (left), and eigenvector features characterized by generalized fractal dimensions (middle and right), for an irreducible Hilbert subspace of a system of 12 bosons in 12 spatial modes.

Hyperbolic light interacting with molecules

Alexey Nikitin
Donostia International Physics Center (DIPC), Donostia-San Sebastián, 20018 Spain
IKERBASQUE, Basque Foundation for Science, Bilbao, 48013 Spain
Email alexey@dipc.org

Phonon polaritons – lattice vibrations coupled to electromagnetic fields – in van der Waals (vdW) materials can enhance light–matter interactions at mid-infrared frequencies, owing to their extreme field confinement and long lifetimes. Particularly, in some vdW crystals (such as in h-BN, MoO_3, V_2O_5 etc) the dispersion of polaritons – the relation between the momentum and energy – can take a hyperbolic shape and lead to the strong coupling between the polaritonic fields and molecular vibrations. In this talk we demonstrate that vibrational strong coupling can be achieved between phonon polaritons either freely propagating along vdW slabs [1] or "locked" inside resonant cavities [2] and molecular vibrations in adjacent thin molecular layers. Such interaction can take place simultaneously in different frequency bands, e.g. at visible and mid-infrared frequencies [3]. We will show the most recent experimental and theoretical studies on the interaction between hyperbolic polaritons and molecules, discuss their applications and future perspectives.

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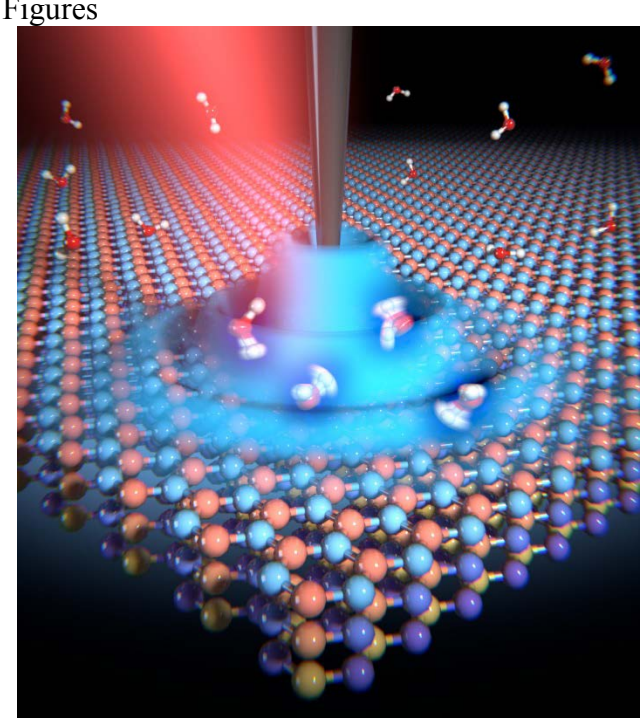

Figure 1: An artistic image of a phonon polariton in h-BN interacting with molecular vibrational resonances. The vertical rod represents the AFM tip of a near-field optical microscope, probing the interaction.

Out of equilibrium dynamical properties of Bose-Einstein condensates in ramped up weak disorder

Rodrigo P A Lima[1,2]
Milan Radonjic[3,4] and Axel Pelster[3]
[1]GISC and GFTC, Instituto de Física, Universidade Federal de Alagoas, Maceió AL, 57072-970,Brazil
[2]Departamento de Fısica de Materiales, Universidad Complutense, E-28040 Madrid, Spain
[3]Physics Department and Research Center OPTIMAS, Technical University of Kaiserslautern, Erwin-Schrödinger Straße 46, 67663 Kaiserslautern, Germany
[4]Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
rodrigo@fis.ufal.br

We investigate theoretically how the superfluid and the condensate deformation[1] of a weakly interacting ultracold Bose gas evolve during the ramping up of an external weak disorder potential. Both resulting deformations turn out to consist of two distinct contributions, namely a reversible equilibrium one, already predicted by Huang and Meng in 1992, as well as a non-equilibrium dynamical one, whose magnitude depends on the details of the ramping protocol. For the specific case of the exponential ramping up protocol, we are able to derive analytic time-dependent expressions for the aforementioned quantities. After sufficiently long time, the steady state emerges that is generically out of equilibrium. We make the first step in examining its properties by studying the relaxation dynamics into it. Also, we investigate the two-time correlation function and elucidate its relation to the equilibrium and the dynamical part of the condensate deformation.

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Quantum plasmonics in monolayer and double layer systems.

Luis Brey
Instituto de Ciencia de Materiales de Madrid (CSIC)
brey@icmm.csic.es

In this contribution we first review the quantization scheme of plasmons in a dissipationless two-dimensional electron gas and extend this formalism to the case of a double layer system coupled by Coulomb interaction. We obtain a quantum Hamiltonian for the double layer plasmons as function of the boson operators of the constituents layers plasmons. By diagonalizing this Hamiltonian, we obtain the optical (in phase) and the acoustic (out of phase) plasmons of the bilayer. Interesting at low momentum and small separation of the layers, the Hamiltonian is in the strong coupling regime and it is crucial to take into account the anti-resonant or counter - rotating terms in order to describe appropriately the plasmons modes of the double layer, in particular the linear dispersion of the acoustic mode.

QUANTUM CAVITIES BASED ON MAGNONIC TEXTURES

María José Martínez-Pérez[1],
Carlos A. González[1], D. García-Pons[1], J. Pérez-Bailón[1], F. Luis[1], D. Zueco[1]
[1]Instituto de Nanociencia y Materiales de Aragón CSIC-Universidad de Zaragoza, Calle Pedro Cerbuna 12, 50009 Zaragoza, España
pemar@unizar.es

Solid state quantum computing and quantum sensing technologies are based on the strong coupling between qubits and a quantized field of excitations. Besides photons, the solid state offers a wide variety of bosonic excitations that can be emitted or absorbed such as, e.g., magnons, the quantum version of spin waves.

Magnonic cavities offer the advantage of operating at reduced wavelengths compared to electromagnetic resonators of the same frequency. Here, we investigate the integration of magnonic cavities based on topological magnetic solitons as, e.g., magnetic vortices. The latter are extremely stable magnetic textures exhibiting a very rich dynamical behavior in the sub-GHz to tens of GHz range. We focus on the coupling of individual spin qubits to vortex cavities for sensing and quantum computing applications.

Model of screening in intrinsic disordered graphene

Marta García Olmos
Universidad de Salamanca, Pl. Caídos, s/n, Salamanca, Spain
mgarcia.o@usal.es

In this work we study the influence of the electron-electron interaction on the low-energy electronic spectrum of graphene with disorder due to non-magnetic impurities. Graphene is a Dirac material that has raised great interest since its discovery due to its unusual electronic properties, and it turns out to be an excellent scenario to analyze the electronic behavior at low dimensionality. On the one hand, the influence of disorder in these systems has been widely studied in the literature. To deal with it we have considered a separable pseudo-potential within the coherent potential approximation formalism. On the other hand, the fact that the density of states cancels out at the Fermi level in these materials implies that the electron-electron interaction remains long-range and its effect on the properties of the system is still unclear. Employing the diagrammatic approximation for electron self-energy we discuss the role played by this interaction on the one-particle properties.

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Clean room processes for 2D materials: side contacts and etching through cryogenic temperature

Vito Clericò
Juan Salvador Sánchez, Marcel Vincente Muñoz, Daniel Vaquero, Abidi El Hadj, Maha Labani, Carlos Sánchez Sánchez, Javier Palazuelo Casquero, Juan Antonio Delgado Notario, Ana Pérez Rodríguez, David López Díaz, José Caridad, Mario Amado, Mercedes Velázquez Salicio, Enrique Velázquez, Yahya Meziani, Enrique Diez

Nanotechnology Group, USAL–Nanolab, Universidad de Salamanca, E-37008 Salamanca, Spain
vito_clerico@usal.es

Some clean room processes on 2D materials are presented, including a detailed description of the whole process (and explanation of the main issues) to obtain a final device [1].
In the last part, we focus the attention on the role of the temperature in a dry etching process. A very controllable etching is fundamental for the realization of side (or edge) contacts in encapsulated 2D materials [2][3][4]. Besides, through the use of cryogenic temperature in the etching process, we were able to obtain nanostructures with very small roughness in comparison with higher etching temperatures. A clear conductance quantization was so observed in encapsulated graphene constriction [5].

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Figures

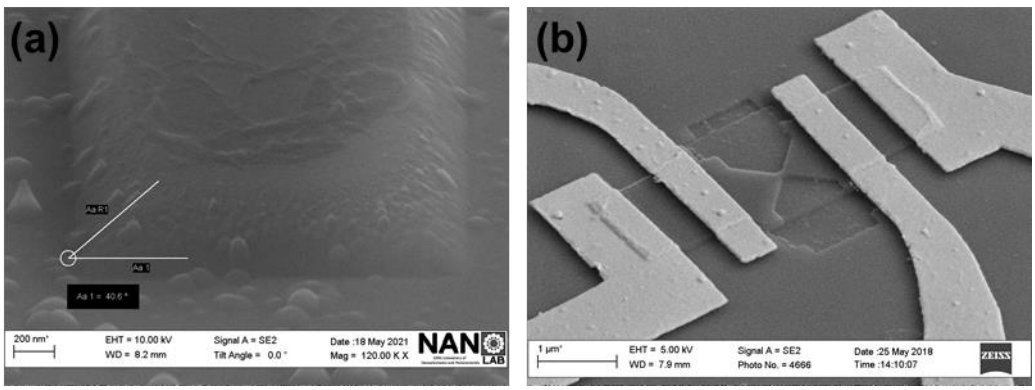

Figure 1: (a) Etching of a (thick) h-BN at 10 °C. (b) Constriction of 100 nm in encapsulated graphene with etching at -110 °C.

Topological states in finite graphene nanoribbons

M. Carmen Muñoz
M. Pilar López-Sancho
Instituto de Ciencia de Materiales de Madrid-CSIC, Cantoblanco, 28049 Madrid, Spain
mcarmen@icmm.csic.es, pilar@icmm.csic.es

We investigate the relation between topologically protected states and the structure of the graphene nanoribbons. By means of calculations based on a Tight-Binding model, the effects of the unit cell edge geometry on the nature of the boundary electronic states are studied. Emergence of topological [1] and confined states in different geometries depends on the structure and width of the ribbons. It is found that sublattice symmetry is on the basis of the appearance of topological phases on graphene nanoribbons [2].

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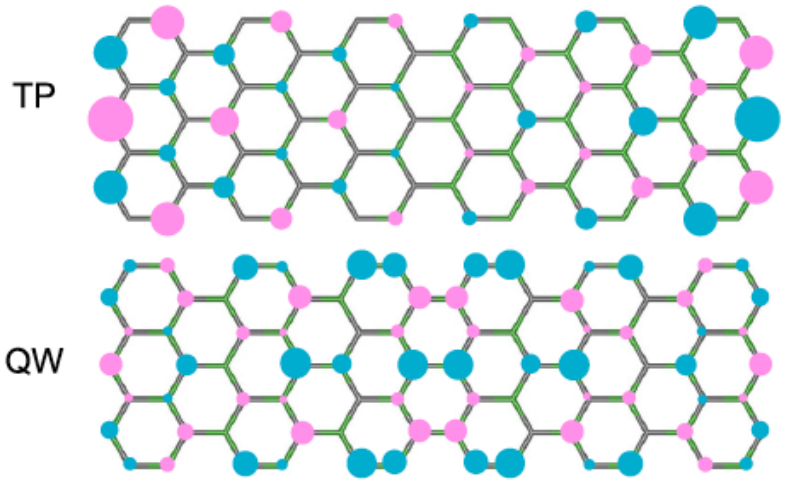

Figure 1: Wave function distribution for the two first occupied states corresponding to an Armchair Graphene Nanoribbon with seven atoms of width. Blue and pink indicate positive and negative amplitudes, respectively.

Scanning Tunneling Spectroscopy in topological Dirac semimetal $ZrTe_5$

Jose Antonio Moreno[1]
Raquel Sánchez-Barquilla[1], Edwin Herrera[1], Isabel Guillamón[1], Hermann Suderow[1]
Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos, Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
josea.moreno@uam.es

$ZrTe_5$ has received much interest as a possible candidate for a topological insulator (TI), which is a new type of quantum matter which features insulating bulk band gaps and is capable of hosting Dirac fermionic states connecting the valence and conduction via Dirac cone bands on its surfaces [1,2]. These exotic properties have shown $ZrTe_5$ to display Quantum Hall Effect among other notable phenomena with interesting application for the development of electronic device applications [3]. The nature of $ZrTe_5$ as a topological insulator has been studied via macroscopic ARPES and microscopic STM measurements. In these, a large 100 meV gap in the conductance was found over the whole surface of the sample and edge states compatible with the observation of Dirac cones were found only on terrace edge steps [4,5]. These results seem to suggest that $ZrTe_5$ surface is a 2D topological insulator, with the bulk material being a weak 3D rather than a Dirac semimetal. In this work, we have synthesized high quality single crystals of $ZrTe_5$ using flux growth. We perform low energy local STM measurements of the electronic density of states. We discuss the tunneling conductance at the surface and around defects. We have applied magnetic fields up to 17 T along the z axis and find peaks on the conductance that might be a signature of Landau levels.

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Electronic band structure and atomic level Landau quantization in the type-II Weyl semimetal WTe_2 visualized by Scanning Tunneling Microscopy

Raquel Sánchez-Barquilla
Francisco Martín-Vega,[1] José J. Baldoví,[2] Masayuki Ochi,[3] Ryotaro Arita,[4] Na Hyun Jo,[5] Sergey L. Bud'ko,[5] Paul C. Canfield,[5], Hermann Suderow[1] and Isabel Guillamón,[1]

[1] *Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos,*
Departamento de Física de la Materia Condensada,
Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC),
Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.
[2] *Instituto de Ciencia Molecular (ICMol), Universidad de Valencia,*
Catedrático José Beltrán 2, 46980 Paterna, Spain.
[3] *Department of Physics, Osaka University, Toyonaka, Osaka 560-0043, Japan.*
[4] *RIKEN Center for Emergent Matter Science, Wako, Saitama 351-0198, Japan*
6Ames Laboratory, Ames, IA 50011.
[5]*Department of Physics & Astronomy, Iowa State University, Ames, IA 50011*

raquel.ranchezb@uam.es

We present scanning tunneling microscopy (STM) measurements at very low temperatures (100 mK) and high magnetic fields (up to 14 T) in the type II Weyl semimetal WTe_2. We obtain the bulk bandstructure by comparing quasiparticle interference (QPI) patterns with detailed Density Functional Calculations (DFT) of surface and bulk states. The bias voltage dependence of the tunneling conductance is not affected by a magnetic field, suggesting that the bandstructure is essentially field independent. We observe however Landau quantization in atomic scale measurements and show the relation to the quantization of electron and hole bands of WTe_2. We show in particular that there is a connection at the surface between electron and hole bands, and that it leads to a modification of the usual sequence of Landau levels.

Next generation, direct X-ray detectors based on perovskite-MOF composites

Hayden Salway[1,2]
Elena Avila[1,], Ganbaatar Tumen-Ulzii,[1] Oliver Moseley[1,2], Nakul Rampal[1], Samuel D. Stranks[1,2], David Fairen-Jimenez[1], Miguel Anaya[1,2,]
[1] *Department of Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom*
[2] *Cavendish Laboratory, University of Cambridge, United Kingdom*
hajs2@cam.ac.uk

Halide perovskites are an exciting family of semiconductors that have seen a tremendous growth in research in photovoltaics and LEDs, owing to their excellent optoelectronic properties including bandgap tunability, high photoluminescence quantum yields (PLQY), defect tolerance and chemical versatility. Similarly, these properties make halide perovskites one of the most promising materials for next-generation, highly sensitive, low-noise, direct X-ray detectors.[1] However, challenges for the successful commercialization of halide perovskites X-ray detectors remain. For example, processing halide perovskites into thick devices for optimal X-ray attenuation, without introducing defects via pressing, or mixing with polymer membranes represents one set of challenges. Further, to realize highly sensitive, low-noise detectors requires novel material choices to reduce dark currents, minimize current drift and enhance stability.

MOFs are another kind of materials which have started the gather attention as promising X-ray detectors, due to their ease of processing and chemical versatility enabling incorporation of high Z atoms maximizing attenuation efficiencies.[2] Besides, recent advancements in sol-gel MOF processing have enabled us to develop high-density monolithic MOF structures through advanced synthesis and densification, resulting in easily size controllable high-density materials.[3]

In this work, we present the first of its kind PVK@MOF direct X-ray detector.[4] Our unique synthesis approach forms halide perovskite nanocrystals via direct conversion from a sol-gel Pb MOF, resulting in size and shape controllable PVK@MOF composite, which can be tailored to the required X-ray energies for applications in Radiography, CT, and PET scanning. The Intrinsically insulating Pb MOF results in a composite with high resistivity, and significant reductions in dark current, whilst maintaining high current densities and sensitivity resulting from charge carriers generated upon X-ray excitation of perovskite nanocrystals within the composite. Moreover, reproducible medical imaging necessitates device resistance to current drift. In this regard, halide perovskites often see large dark current drifts, due to strong ion migration effects, thus requiring long pre-biasing before optimally functioning. However, our PVK@MOF composite shows a significant reduction in dark current drift compared to the equivalent standalone perovskite detector, which we attribute to the rigid MOF structure limiting ion migration effects. We further present a full direct X-ray detector material characterisation framework using our PVK@MOF composite, demonstrating the full range of device performances which can be achieved by varying incident properties. The methodology within this work will lay the foundations for further device performance characterisation, removing ambiguity from current performance metrics, giving potential to significantly advance the application and commercialisation of halide perovskite X-ray detectors.

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Bulk photovoltaic effect in 2D materials from density functional theory and real-time dynamics

J.J. Esteve-Paredes[1], M. Malakhov[2], A. Uría[1], G. Cistaro[2] , A. Picón[2] and J.J. Palacios [1,3]
[1]*Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain.*
[2]*Departamento de Química, Universidad Autónoma de Madrid, Madrid, Spain.*
[3]*Instituto Nicolás Cabrera (INC) and Condensed Matter Physics Center (IFIMAC).*
Email: juan.esteve(at)uam.es

The bulk photovoltaic effect (BPVE) is a phenomenon that consists in the generation of a DC current in a material under ilumination with strong enough oscillating electric fields. This effect is intrinsic and occurs in non-centrosymmetric materials without the need of heterostructures or interfaces. The second-order current that contributes to the BPVE is known as the shift-current. First-principles Density Functional Theory (DFT) calculations of this quantity have been carried out during the last decade, seeking efficient materials that can be used for solar energy conversion. In this talk, we present two DFT-based methodologies to evaluate the first and second-order (DC) responses based on (i) evaluating the frequency-dependent perturbative expressions and (ii) soving the time-dynamical equations for the density matrix incuding an electric pulse. The use of Gaussian basis sets saves computational effort, where typical expressions containing expensive “sums over bands” become expeditious. More remarkably, our time-dynamics approach allows to include electron-hole effects in the calculation of shift currents, a theoretical challenge with almost no general understanding yet. We apply our methodology to several 2D crystals that elucidate the enormous changes in the shift-current, inlcuding both a huge redshift in energy and qualitative changes in its shape, when one goes beyond a single-particle DFT approach.

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Large topological Hall effect and spin textures in $La_{0.7}Sr_{0.3}MnO_3$ / $SrIrO_3$ bilayers

Andrea Peralta-Somoza[1]
Sandra Lopez[1] J.J. Riquelme[3,4], I. Barbero[1], Javier Tornos[1], Víctor Zamora[1], F. A. Cuellar[1] Sergio Valencia[2], C. Munuera[3,4], F. Mompeán[3,4], M. García-Hernández[3,4], C. León[1] and Jacobo Santamaría[1]
[1] *GFMC, Dept. Fisica de Materiales, Facultad de Fisica, U. Complutense, 28040 Madrid, Spain.*
[2] *Helmholtz Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany*
[3] *2D-Foundry Group, I.de Ciencia de Materiales de Madrid ICMM-CSIC, 28049 Madrid, Spain*
[4] *Laboratorio de Heteroestructuras con Aplicación en Espintrónica, ICMM-CSIC, Madrid, Spain*
anperalt@ucm.es

Magnetic skyrmions and other topologically protected spin textures have gained interest as they can be used as low-power information vectors. Spin textures can be stabilized by the interplay between exchange interaction, promoting parallel spin alignment, and Dzyaloshinskii-Moriya interaction, an antisymmetric exchange interaction resulting from the combination of inversion symmetry breaking and strong spin-orbit coupling, which twists spin directions. Although skyrmions or skyrmion bubbles have been found in non-centrosymmetric single magnetic oxide layers [1], interfaces naturally provide symmetry breaking and promote the generation of spin textures in heterostructures [2,3]. Non-trivial topological charge of skyrmions gives rise to antisymmetric transverse resistivity, the so-called topological Hall effect, THE. Whether THE results from spin chirality or from magnetic inhomogeneity has become an actively debated matter [4,5], boosted by the fact, that, frequently, reports of the THE are not accompanied by real space imaging of the magnetic textures. In this work we report large THE in bilayers combining ultrathin $La_{0.7}Sr_{0.3}MnO_3$ and strong spin orbit $SrIrO_3$ in a wide temperature range. Real space observations of the magnetic textures by magnetic force microscopy (MFM) and photoemission microscopy using x-ray magnetic circular dichroism contrast (PEEM) evidence a coarsened small grain (100 nm) magnetic structure inferred from image analysis, consistent with the nucleation and clustering of skyrmions or skyrmion bubbles. Field cool in strong magnetic fields above 5T suppress the THE signal and consistently the MFM contrast of the magnetic textures, suggesting the possibility to control the skyrmions. Magnetometry and anomalous Hall effect will be discussed to infer the relative importance of magnetic inhomogeneity.

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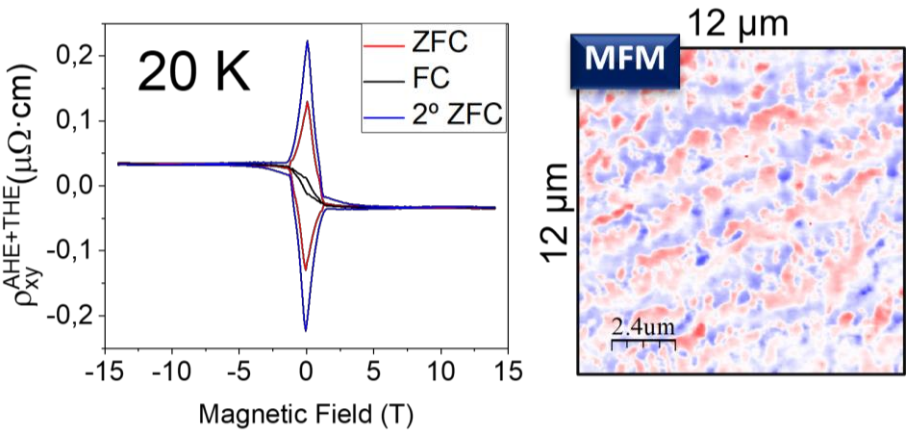

Figure 1: Left panel. Anomalous Hall effect measured at 20 K after field cooling (FC) (black line) and zero field cooling (ZFC) (red and blue lines). Right panel. MFM image at 17 K after ZFC.

Focusing of In-plane Hyperbolic Polaritons in Van der Waals Crystals

Javier Martín-Sánchez[1,2]
Jiahua Duan[1], Javier Taboada-Gutiérrez[1,2], Gonzalo Álvarez-González,[1,2], Kirill V. Voronin[3], Iván Prieto[4], Weiliang Ma[5], Qiaoliang Bao[5], Valentyn S. Volkov[3], Rainer Hillenbrand[6,7], Alexey Y. Nikitin[3], Pablo Alonso-González[1,2]
[1]*Departamento de Física, Universidad de Oviedo, Oviedo, Spain*
[2]*Nanomaterials and Nanotechnology Research Center (CINN-CSIC), El Entrego, Spain*
[3]*Donostia International Physics Center (DIPC), Donostia/San Sebastián, Spain*
[4]*Institute of Science and Technology Austria IST, Am Campus 1, 3400 Klosterneuburg, Austria*
[5]*Huazhong University of Science and Technology, Wuhan, China*
[6]*nanoGUNE BRTA and Department of Electricity and Electronics, UPV/EHU, Spain*
[7]*Donostia International Physics Center (DIPC), Donostia-San Sebastián, Spain.*
javiermartin@uniovi.es

Polaritons -hybrid light-matter excitations- play a crucial role in fundamental and applied sciences, as they enable control of light on the nanoscale [1]. The recent emergence of low-loss van der Waals (vdW) materials opens the door to achieving anisotropic optical phenomena owing to their layered crystal structure, which leads to an intrinsic and strong out-of-plane (perpendicular to the layers) optical anisotropy. A prominent example is given by hyperbolic phonon polaritons (PhPs) -infrared light coupled to lattice vibrations in layered polar materials- in hexagonal boron nitride (h-BN) [2], which exhibit long lifetimes, ultra-slow propagation and hyper-lensing effects. Only recently, PhPs with in-plane hyperbolic dispersion, a key requirement for on-chip planar optical circuitry, have been demonstrated in natural slabs of α-phase molybdenum trioxide (α-MoO3) [3-5] and vanadium pentaoxide (α-V2O5) [6].

In this work, we demonstrate focusing of infrared ray-like hyperbolic PhPs into deep subwavelength focal spots along the surface of α-MoO3 crystals by using metal antennas with an optimized design. Specifically, field confinement is achieved in focal spots with a size of λp/4.5=λ0/50 (λp is the polariton wavelength and λ0 is the photon wavelength in free space). Moreover, the achievable focal distance in in-plane hyperbolic α-MoO3 can be tuned to values well below the diffraction limit in in-plane isotropic materials, along with a better performance in terms of near field confinement and optical absorption. Our findings set the grounds for planar polaritonic technologies at the nanoscale [7].

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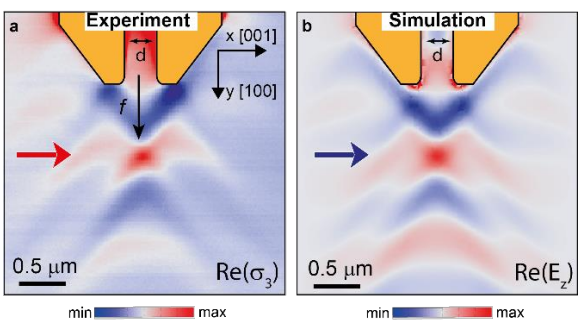

Fig. 1 Nanofocusing of PhPs along the surface of a α-MoO_3 flake into deep-subwavelength focal spots.

Li-Diffusion processes through Carbon Nanotube / Graphene interfaces: anode material for solid-state battery application

Hernán Santos[1]
Emerick Guillaume[2], María Sánchez, Luc Henrard[2], and Alejandro Ureña[1]

[1]*Dept. de Matemática Aplicada, Ciencia e Ingeniería de Materiales y Tecnología Electrónica, ESCET, Universidad Rey Juan Carlos, C/ Tulipán s/n, 28933 Móstoles, Madrid, Spain*
[2]*Department of Physics and Namur Institute of Structured Materials, University of Namur, Rue de Bruxelles 61, 5000 Namur, Belgium*
hernan.santos@urjc.es

We investigate the Li diffusion through carbon nanotube (CNT) - graphene interface channels by Density Functional Theory calculations including van der Waals interaction and using the climbing nudge elastic band (cNEB) method. We have found an enhanced mobility of Li ions over graphene when carbon nanotube is present. The bilayer area between CNT and graphene acts as a well of the surface energy potential (SEP) that traps Li atoms, which moves with high mobility over graphene towards this area [1]. Moreover, the increased charge transfer from Li located in the bilayer area modifies and increases the chemical potential and therefore the capacity of batteries. This model with an alternate bi-layer and one-layer graphene account for the modified carbon fiber decorated with CNT employed as anode electrode material in solid-state batteries and structural supercapacitors [2], explaining its enhanced capacity and increased ionic conductivity.

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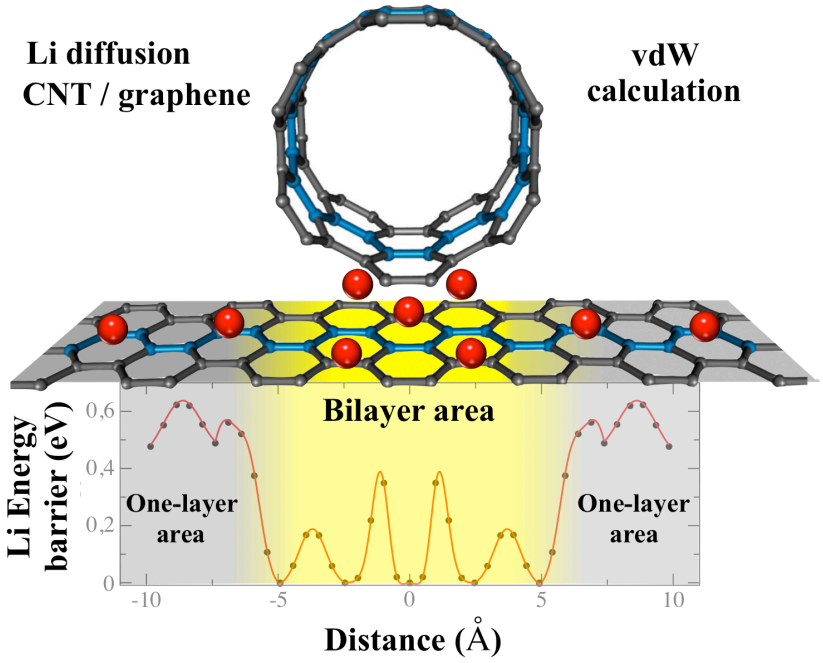

Figure 1: Energy barriers of Li along different paths over grafene / CNT heterostructure by NEB VASP calculation.

A coarse-grained approach for growth simulations of metal oxides and polymers on planar/nanostructured substrates

Jorge A. Budagosky M., 1,2 *
Xabier García-Casas,1 J. R. Sánchez-Valencia,1 Ángel Barranco,1 Ana Borrás,1**
1 *Nanotechnology on Surfaces and Plasma Group, Materials Science Institute of Seville (CSIC-US), Seville, Spain.*
2 *Department of Applied Physics I, Higher Polytechnic School, University of Seville, Seville, Spain.*
(*) jbudagosky@us.es, (**) anaisabel.borras@icmse.csic.es

Thin films growth on both flat and nanostructured substrates is studied by means of a coarse-grained kinetic Monte Carlo simulation under conditions typically encountered in Plasma Enhanced Chemical Vapor Deposition experiments. The basis of our approach is known to work well to simulate the growth of amorphous materials using cubic grids and have been extended here to reproduce not only the morphological characteristics and scaling properties of amorphous TiO2 but also the growth of materials with very different structural characteristics, like polycrystalline wurtzite-type ZnO and plasma polymers [1]. The results of the simulations have been compared with available experimental data obtained by X-Ray Diffraction, analysis of the texture coefficients, Atomic Force Microscopy, and Scanning Electron Microscopy. The model is shown to reproduce with a good approximation many relevant features of the real samples.

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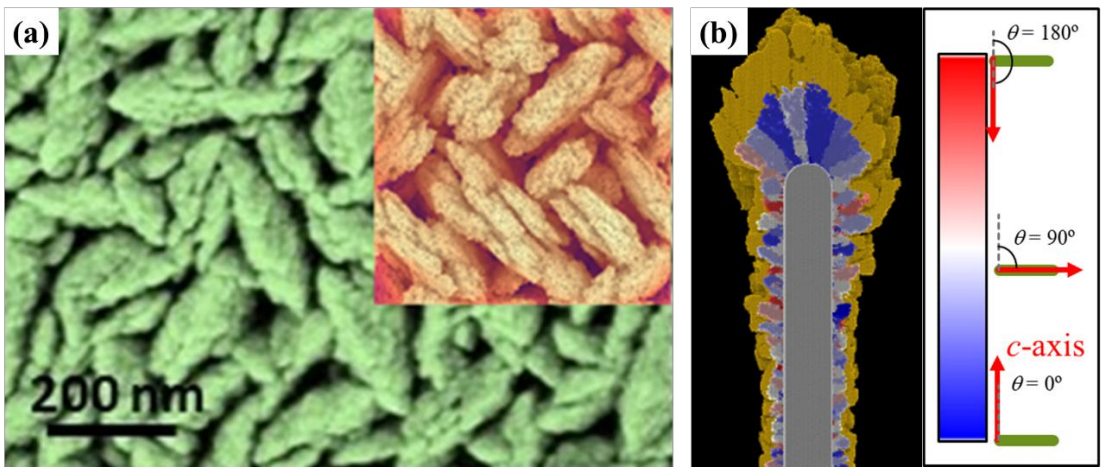

Figure 1: (a) Top-view Scanning Electron Microscopy micrograph of a wurtzite-type ZnO film with nanocolumnar morphology fabricated by PECVD on Si substrates at RT conditions under oxygen plasma and growth rate of 10 nm/min. The inset is the simulated thin-film morphology obtained by assuming similar growth conditions. (b) Longitudinal cut of a simulated ONW@ZnO@SiO_2 core@multishell nanowire growth under PECVD conditions. The color scale shows the c-axis orientation of the different grains forming the inner ZnO shell.

Mechanical and acoustic properties of graphene explained thanks to anharmonic effects

Presenting Author: Josu Diego
Co-Authors: Unai Aseginolaza, Tommaso Cea, Raffaello Bianco, Lorenzo Monacelli, Matteo Calandra, Aitor Bergara, Francesco Mauri and Ion Errea
Affiliation, Address, City, Country:
University of the Basque Country (UPV/EHU), Donostia-San Sebastián, Spain
Centro de Física de Materiales (CSIC-UPV/EHU), Pº Manuel de Lardizabal 5, Donostia-San Sebastián, Spain
Email: josu.diego@ehu.eus

The phonon properties of graphene, and in general of any 2D material, are still highly debated. The harmonic approximation predicts diverging atomic fluctuations and a constant linewidth of in-plane acoustic phonon modes at small momentum, which implies that graphene cannot propagate sound waves. The origin of these problems is the quadratic dispersion of the acoustic out-of-plane phonon frequencies obtained in the harmonic approximation. By including anharmonicity in a non-perturbative way within the Stochastic Self-Consistent Harmonic Approximation (SSCHA) we show that the physical dispersion expected experimentally for the acoustic out-of-plane mode should indeed be quadratic but actually compatible with well-defined sound waves. We verify this result using both atomistic simulations and a membrane model for graphene.

We also focus on the nature of the ripples by analyzing wihin the membrane model the scaling of the equal time out-of-plane correlation function. Our results replicate the crossover from classical correlations to quantum ones reported by Hašík et al. through quantum PIMC simulations [2]. We also suggest that most works in the membrane based literature [3] are conditioned by the non-rotationally invariance of their model.

Our conclusions [1] not only have a crucial role in the understanding of the mechanical and acoustic properties of graphene, but also of other strictly two-dimensional material.

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Multiple and spectrally robust photonic magic angles in reconfigurable α-MoO3 trilayers

Presenting Author (Aitana Tarazaga Martín-Luengo[1,2])

J. Duan1,[2,†], G. Álvarez-Pérez[1,2], C. Lanza[1,2], A.I.F. Tresguerres-Mata[1,2], K. Voronin[3], N.Capote-Robayna[3], J. Martín-Sánchez[1,2], V.S. Volkov[4,5], A.Y. Nikitin[3,6,†], and P. Alonso-González[1,2,†])

[1] *Department of Physics, University of Oviedo, Oviedo 33006, Spain.*
[2] *Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo), El Entrego 33940, Spain.*
[3] *Donostia International Physics Center (DIPC), Donostia-San Sebastián 20018, Spain.*
[4] *Center for Photonics and 2D Materials, Moscow Institute of Physics and Technology, Dolgoprudny, 141700, Russia.*
[5] *GrapheneTek, Skolkovo Innovation Center, Moscow, Russia.*
[6] *IKERBASQUE, Basque Foundation for Science, Bilbao 48013, Spain.*
[†] *Corresponding to: duanjiahua@uniovi.es, alexey@dipc.org, pabloalonso@uniovi.es)*
Email (aitanatarazaga@uniovi.es)

The assembling of twisted stacks of van der Waals (vdW) materials had led to the discovery of a profusion of remarkable physical phenomena in recent years, as it provides a means to accurately control and harness electronic band structures. This has given birth to the so-called field of twistronics. An analogous concept has been developed for highly confined polaritons [1][2], or nanolight, in twisted bilayers of strongly anisotropic vdW materials [3], extending the field to the twistoptics realm. In this case, the emergence of a topological transition of the polaritonic dispersion at a given twist angle (photonic magic angle) results in the propagation of nanolight along one specific direction (canalization regime), holding promises for unprecedented control of the flow of energy at the nanoscale. However, there is a fundamental limitation in twistoptics that critically impedes such control: there is only one photonic magic angle (and thus canalization direction) in a twisted bilayer and it is fixed for each incident frequency. Here, we overcome this limitation by demonstrating the existence of multiple spectrally robust photonic magic angles in reconfigurable twisted vdW trilayers.

As a result, we show that **canalization of nanolight can be programmed at will along any desired in-plane direction in a single device**, and, importantly, **within broad spectral ranges** of up to 70 cm^{-1}. Our findings lay the foundation for robust and widely tunable twistoptics, opening the door for applications in nanophotonics where on-demand control of energy at the nanoscale is crucial, such as thermal management, nanoimaging or entanglement of quantum emitters.

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Accurate transfer of individual nanoparticles onto single photonic nanostructures

J. Redolat [1]
M. Camarena-Pérez[1], A. Griol[1], M. Kovylina[1], A. Xomalis[2,3], J. J. Baumberg[2], A. Martínez[1] and Elena Pinilla-Cienfuegos[1*]
[1] *Universitat Politècnica de València, Nanophotonics Technology Center, Valencia E46022, Spain*
[2]*NanoPhotonics Centre, Cavendish Laboratory, Department of Physics, JJ Thompson Avenue, University of Cambridge, Cambridge CB3 0HE, United Kingdom*
[3]*Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Thun, Switzerland*
E-mail: epinilla@ntc.upv.es

Controlled integration of metallic nanoparticles (NPs) onto photonic nanostructures enables realization of complex devices for extreme light confinement and enhanced light-matter interaction. Extreme light confinement can be achieved combining Nanoparticle-on- Mirror (NPoM) nanocavities [1-2] with the light manipulation capabilities of micron-scale metallic antennas and/or photonic integrated waveguides [3]. However, metallic NPs are usually deposited via drop-casting, which prevents their accurate positioning. Here we present a methodology for precise transfer and positioning of individual NPs onto different photonic nanostructures. The method is based on soft lithography printing that employs elastomeric stamp-assisted transfer [4] of individual NPs onto a single nanostructure. It can also parallel imprint many individual NPs with high throughput and accuracy in a single step. Raman spectroscopy confirms enhanced light-matter interactions in the resulting devices. Our method mixes *top-down* and *bottom-up* nanofabrication and shows the potential of building complex photonic nanodevices for applications ranging from enhanced sensing and spectroscopy to signal processing.

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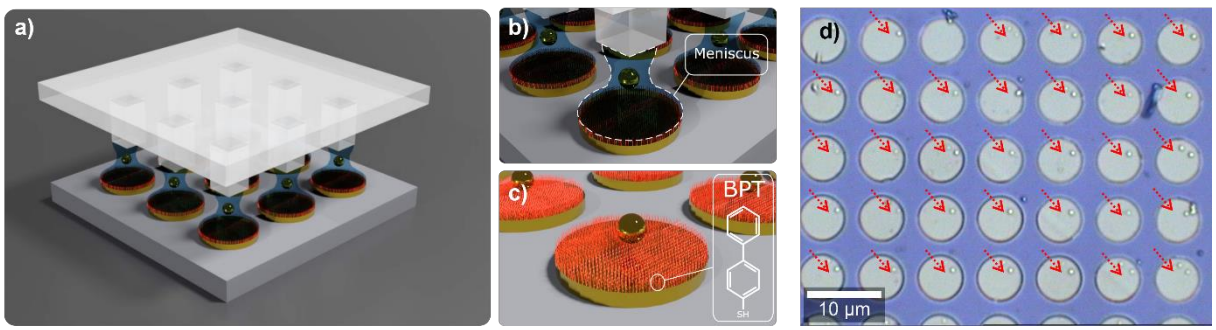

Figure 1. a) Schematic parallel stamp-assisted printing method. b) Meniscus formation between the stamp protrusion and sample. c) BPT Functionalized lithographed Au sample with NP attached. d) Optical image of a Au/BPT disk array after single-step NP transfer. Red arrows show NP positioning**.**

Interaction-driven Circular Dichroism through absorption modes in Triskelia Nanostructures

Javier Rodríguez-Álvarez[1,2]
Antonio García-Martín[3], Arantxa Fraile Rodríguez[1,2], Xavier Batlle[1,2], and Amílcar Labarta[1,2]
1 Departament de Física de la Matèria Condensada, Universitat de Barcelona, 08028 Barcelona, Spain
2 Institut de Nanociència i Nanotecnologia (IN2UB), Barcelona, 08028, Spain
3 Instituto de Micro y Nanotecnología IMN-CNM, CSIC, CEI UAM+CSIC, Isaac Newton 8, E28760 Tres Cantos, Madrid, Spain
javier.rodriguez@ub.edu

Our work is focused on the design, simulation and manufacture of a simple 3D structure that presents large CD in the near-Infrared (NIR) and optical ranges that can be easily tuned by adjusting its geometrical parameters [1].
The building block used in this work, so-called "triskelion", shows a three-fold rotational symmetry and has chiral nature (Figure 1c). A single triskelion shows significant dichroism in both the absorption and scattering (Figure 1a and 1b). However, the two dichroic signals cancel each other owing to its planar nature [2]. On the contrary, our simulations reveal that the two triskelia system presents a dichroic signal in the extinction. The arising dichroism is mainly due to two extra excitations, not present in the single triskelion case, exhibited by the absorption at wavelengths greater than 0.7 and 1.1 μm, respectively. Furthermore, the position of these two peaks can be shifted by changing either the edge-to- edge distance between the triskelia or their relative angle of rotation. This strongly supports the fact that these additional excitations are caused by the interactions between the two triskelia. Such shifting enables an accurate control of both the wavelength ranges at which the CD appears and its sign, providing a simple platform to finely control the CD of the system by adjusting the distance between the triskelia and their relative rotation angle, two parameters that can be easily tuned in the manufacturing process.

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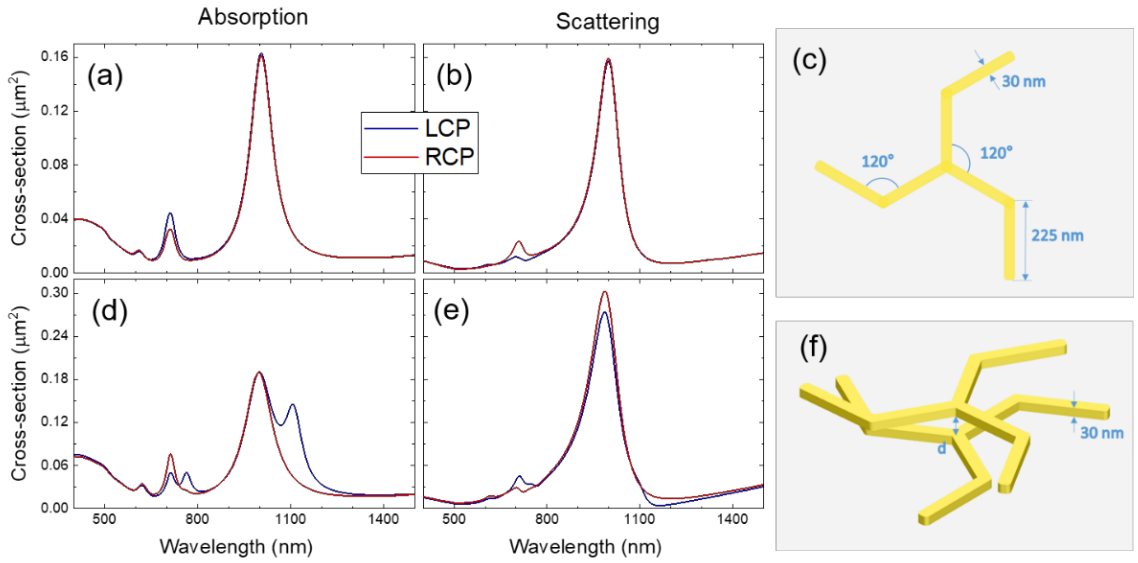

Figure 1. Absorption (a) and scattering (b) cross-section spectra for a single triskelion, and (d) and (e) two triskelia with a relative rotation angle of 30° and 30 nm of separation. Right panels (c) and (f) show schematic representations of a single triskelion and two triskelia, respectively.

Vortex lattice at high magnetic fields and charge density wave in $KCaFe_4As_4$ and $CaK(Fe_{0.988}Mn_{0.012})$

Marta Fernández Lomana, [1] Beilun Wu,[1] Hermann Suderow[1], Young-Joon Song[2], Roser Valentí[2], William Meier, Andreas Kreyssig, Sergey L. Bud'ko,[3] Paul C. Canfield,[3] and Isabel Guillamon[1]

1 Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos,
Departamento de Física de la Materia Condensada,
Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC),
Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.
2Institute for Theoretical Physics, Goethe University Frankfurt,
Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany.
3Department of Physics & Astronomy, Iowa State University, Ames, IA 50011
marta.fernandez-lomana@uam.es

The 1144 CaKFe4As4 compound is a pnictide superconducting material showing optimal superconducting critical temperature with Tc as large as 38 K [1,2]. There are no signatures of nematic, structural or magnetic transitions. Doping with Ni and Mn induces a decrease in Tc and the appearance of magnetism. Instead of the stripe like spin density wave (SSDW) antiferromagnetic order present in the 122 systems, Ni and Mn-doped CaKFe4As4 shows a spin vortex (or hedgehog) magnetic order [3,4]. This is due to the lack of glide symmetry in the FeAs plane of the crystalline structure of the 1144 compounds. Here we present scanning tunneling microscopy experiments in pure, Ni-doped and Mn-doped CaKFe4As4. We have determined the superconducting density of states and observed the vortex lattice at very high magnetic fields up to 20 T. Atomic scale measurements show the appearance of a charge density wave order (CDW) induced by the magnetic field in CaKFe4As4 above 10 T, which is also observed in the magnetic Ni and Mn-doped compounds at lower magnetic fields. The CDW has a periodicity of $\sqrt{2}a0 \times \sqrt{2}a0$ where $a0$ is the lattice parameter. Our results suggest that Hedgehog magnetic order is accompanied by an asymmetric displacement of the of the As atoms giving rise to a CDW [5] and that the magnetic field reinforces Hedgehog antiferromagnetic correlations.

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