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XII REUNIÓN DE LA DIVISIÓN DE FÍSICA **DE LA MATERIA CONDENSADA**

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GEFES2023

1-3 Febrero

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70-157 POSTER SESSION A

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PROGRAMME

TUESDAY, JANUARY 31st

- 12:30 Scientific outreach talks:
Rebeca Palau-Ribeiro (CN2-Paris-Saclay): COLEGIO MARISTAS
Esther Barrena (ICMAB-CSIC-Barcelona): IES LUCÍA DE MEDRANO
Elena Pinilla (UPV-Valencia): IES MATEO HERNÁNDEZ
Ana Pérez-Rodríguez (USAL, Salamanca): IES CALISTO Y MELIBEA

- 20:30 **GEFES2023 WELCOME PARTY:** Sala de Pinturas – Colegio Fonseca

WEDNESDAY, FEBRUARY 1st

MORNING SESSION

- 8:00 Registration desk opening: Hospedería Fonseca

- 9:00 **GEFES2023 Opening: Auditorio, Hospedería Fonseca**

2D Materials I

Chair:
Francisco Domínguez-Adame
(Univ. Complutense, Madrid)

- 9:15 Keynote: **Rebeca Ribeiro (C2N Paris-Saclay and CNRS)**
Non-identical moiré twins in bilayer graphene
- 10:00 Invited: **Pablo Ares (Universidad Autónoma de Madrid)**
Piezoelectricity and ferroelectricity in hexagonal boron nitride
- 10:20 Invited: **Fernando de Juan (Donostia International Physics Center)**
Magnetic Kondo lattices in two dimensional metallic dichalcogenides
- 10:40 **Carmen Rubio (Freie Universität Berlin)**
Universal moiré nematic phase in twisted graphene

- 11:00 COFFEE BREAK AND POSTER SESSION A1

2D Materials II

Chair:
Blanca Biel
(Universidad de Granada)

- 12:00 Invited: **Juan A. Delgado-Notario (Universidad de Salamanca)**
Graphene field effect transistors for THz technology and applications
- 12:20 Invited: **Marco Gobbi (CIC-NANOGUNE, Donostia)**
Non-reciprocal charge transport in chiral Tellurium nanowires
- 12:40 **María Rodríguez-Losada (Universidad de Granada)**
Non-perturbative indirect exchange in spin-valley coupled 2D crystals
- 13:00 **Olga Arroyo (ICMM-CSIC, Instituto de Ciencia de Materiales de Madrid)**
Universality of moiré physics in collapsed chiral carbon nanotubes

- 13:20 CONFERENCE PICTURE: COLEGIO FONSECA

- 13:30 LUNCH

WEDNESDAY, FEBRUARY 1st

AFTERNOON SESSION

Soft Matter

Chair:
Alberto Fernández Nieves
(Universitat de Barcelona)

- 15:00 Keynote: **Olivier Dauchot (ESPCI CNRS – Paris)**
When active matter turns solid: from collective motion to collective
- 15:45 Invited: **Laura Rodríguez Arriaga (Universidad Autónoma de Madrid)**
Rotating vesicles to mimic cell motion
- 16:05 **Arturo Moncho-Jordá (Universidad de Granada)**
Non-equilibrium active switching of soft colloids: microstructure, phase behaviour and heterogeneous dynamics
- 16:25 **Javier Rojo-González (Universitat de Barcelona)**
Nematics in solid tori: Doubly twisted structures and defect populated configurations

16:45

COFFEE BREAK AND POSTER SESSION A2

Nanophotonics I

Chair:
Elena Piñilla
(Universitat Politècnica de València)

- 17:45 Keynote: **Alejandro Manjavacas (Instituto Daza de Valdés CSIC)**
Lattice resonances: a collective response of periodic arrays of nanostructures
- 18:30 Invited: **Paloma Arroyo Huidobro (University of Lisbon)**
Temporal and spatio-temporal metamaterials
- 18:50 **Daniel Vaquero (Universidad de Salamanca)**
Fast response photogating in monolayer MoS2 phototransistor
- 19:10 **Javier Rodríguez-Álvarez (Universitat de Barcelona)**
Imaging of Anti-ferroelectric Dark Modes in an Inverted Plasmonic Lattice

THURSDAY, FEBRUARY 2nd

MORNING SESSION

Spintronics and Magnetism

Chair:
Luis López
(Universidad de Salamanca)

- 9:00 Keynote: **Jairo Sinova (Inspire Group, University of Mainz)**
The emergence of research landscape of altermagnetism
- 9:45 Invited: **Sandra Ruiz Gómez (Max Planck Institute for Chemical Physics of Solids, Dresden)**
Direct x-ray detection of the Spin Hall Effect
- 10:05 Invited: **José Hugo García (ICN2-Institut Català de Nanociència i Nanotecnologia, Barcelona)**
Electronic control of spin currents in low-symmetry transition metal dichalcogenides
- 10:25 **Jaume Meseguer (ICMOL, Universitat de València)**
Coexistence of structural and magnetic phases in van der Waals magnet CrI₃
- 10:45 **Alexandru Delamoreanu (Oxford Instruments)**
Cryogenics for Quantum Technology and Condensed Matter Physics

11:05

COFFEE BREAK AND POSTER SESSION B1

Nanophotonics II

Chair:
Pablo Alonso
(Universidad de Oviedo)

- 12:00 Invited: **Rui E. F. Silva (ICMM-CSIC, Instituto de Ciencia de Materiales de Madrid)**
Strong field phenomena in solids
- 12:20 Invited: **Elena Pinilla (Universitat Politècnica de València)**
Optical bistability based on the integration of a molecular nanomaterial in silicon photonics
- 12:40 **Sungguen Ryu (IFISC-CSIC, Universitat de les Illes Balears)**
Periodically driven chiral engine beyond the Carnot limit
- 13:00 **Javier Martín (Universidad de Oviedo)**
Focusing of In-plane Hyperbolic Polaritons in Van der Waals Crystals

13:20

LUNCH

AFTERNOON SESSION

Novel Devices and Functionalities

Chair:
José María De Teresa
(INMA-Univ. Zaragoza)

- 15:00 Invited: **Beatriz Martín García (CIC-NANO GUNE, Donostia)**
Layered hybrid metal-halide perovskites under strain: insights from photoluminescence and micro-Raman spectroscopy
- 15:20 Invited: **Javier del Valle (University of Geneva)**
Fundamentals and applications of the voltage-triggered insulator to metal transition
- 15:40 Invited: **Sara Lafuerza Bielsa (INMA - Universidad de Zaragoza)**
Investigating new electrocaloric oxides for sustainable and efficient refrigeration applications
- 16:00 **Sergio Puebla (ICMM-CSIC, Instituto de Ciencia de Materiales de Madrid)**
Combining Freestanding Ferroelectric Perovskite Oxides with Two-Dimensional Semiconductors for High Performance Transistors

Best Paper and PhD Awards Session

Chair:
Julia Herrero
(INMA-Univ. Zaragoza)

- 17:20 Best Paper Award: **David Sánchez-Manzano (CNRS-Thales, Palaiseau)**
Extremely long-range, high-temperature Josephson coupling across a halfmetallic ferro-magnet
- 17:50 Best Experimental PhD: **Francesco Callavalle (CIC Nanogune – Donostia)**
Probing and tuning the electronic properties of low dimensional Van der Waals materials
- 18:10 Best Theoretical PhD : **Iñigo Robredo Magro (University of the Basque Country)**
Topological Materials from a Symmetry Perspective
- 18:30 Best Theoretical PhD: **Oscar Pozo Ocaña (Materials Physics Center, Donostia)**
On symmetry and topological aspects of novel phases of matter

19:30

GUIDED TOUR around Salamanca old town including Escuelas Mayores

21:00

CONFERENCE **COCKTAIL-DINNER** at Casino de Salamanca (Palacio de Figueroa) – C/ Zamora 11

FRIDAY, FEBRUARY 3rd

MORNING SESSION

Quantum Materials and Technologies

Chair:
Ramón Aguado
(ICMM-CSIC, Madrid)

- 9:00 Keynote: **Natalia Ares (Oxford University)**
Quantum devices for thermodynamics at the nanoscale
- 9:45 Invited: **Edwin Herrera (Universidad Autónoma de Madrid)**
Visualizing waves and quantum well states at the surface of the heavy fermion URu₂Si₂
- 10:05 Invited: **Daniel Gosálbez-Martínez (Universidad de Alicante)**
Diversity of radial spin textures in chiral materials
- 10:25 **Katerina Vaxevani (CIC-NANOGUNE, Donostia)**
Extending the spin excitation lifetime of a magnetic molecule on a proximitized superconductor
- 10:45 **Toraya Fernández (Universidad de Cantabria, Santander)**
Real-Time Second Principles TD-DFT calculations of Optical Properties:
Can large-scale methods be used to simulate Excitons?

11:05

COFFEE BREAK

Nanomaterials

Chair:
Arantxa Fraile
(Universitat de Barcelona)

- 11:35 Keynote: **Irene Calvo (INMA – CSIC , University of Zaragoza)**
Synchrotron X-ray Coherence to Probe the Complexity of realistic interfaces at the Nanoscale
- 12:20 Invited: **Lourdes Marcano (Universidad de Oviedo)**
Quantifying the magnetic anisotropy of 50 nm-magnetic nanoparticles embedded in biological entities
- 12:40 Invited: **Ana Isabel Borrás (ICMSE-CSIC Instituto de Ciencia de Materiales de Sevilla)**
Nanogeneratos and self-powered sensors enable by plasma and vacuum processing of multifunctional thin films and 3D nanoarchitectures
- 13:00 **Tamara de Ara (Universidad de Alicante)**
STM Study and Electronic Transport Signature of Dithiahelicenes at Ambient Conditions
- 13:20 **Noa Varela (Universidade de Santiago de Compostela)**
Spatial control of the thermal conductivity in transition metal oxides

13:40

POSTER AWARDS AND CLOSING CEREMONY

14:00

JUNTA GENERAL GEFES



SPEAKERS

Non-identical moiré twins in bilayer graphene

Rebeca Ribeiro-Palau

Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies (C2N), 91120 Palaiseau, France
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The superlattice obtained by aligning a monolayer graphene and boron nitride (BN) inherits from the hexagonal lattice a 60° periodicity with the layer alignment. This implies that the mechanical, optical and electronic properties of the heterostructure must be identical for 0° and 60° of layer alignment. Surprisingly, this periodicity apply only for the monolayer case. In this talk, I will show you that the moiré superlattice formed by a bilayer graphene aligned with BN, is present every 60° , but the symmetry is broken between the 0° and 60° alignments, creating non-identical moiré twins with different electronic properties. In particular, electron transport measurements display a fully developed valley Hall effect at 0° while it is completely absent at 60° . The origin of the non-identical moiré twins is explained by studying the relaxation of the atomic structures using state-of-the-art numerical techniques, which highlight the central role of the Bernal stacking configuration with respect to the BN layer. Our results challenge the current understanding of the valley Hall effect, since a simple Berry curvature argument do not hold to explain this 120° periodicity in bilayer graphene/BN. This unique interplay between mechanical and electronic properties, demonstrated by the in situ control of the rotational order, increases the possibilities for band-structure engineering on van der Waals heterostructures.

Piezoelectricity and ferroelectricity in hexagonal boron nitride

Pablo Ares^{1,2†}

Colin R. Woods^{1,2}, Tommaso Cea³, Yi Bo Wang^{1,2}, Matthew. J. Holwill^{1,2}, Harriet Nevison-Andrews^{1,2}, Rafael Roldán⁴, Daria V. Andreeva⁵, René Fabregas¹, Neils R. Walet¹, Andre K. Geim^{1,2}, Francisco Guinea^{1,3}, Konstantin S. Novoselov^{1,2}, Laura Fumagalli^{1,2}

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Two-dimensional (2D) hexagonal boron nitride (hBN) is a wide-bandgap van der Waals crystal with a unique combination of properties, including a honeycomb lattice very close to that of graphene, exceptional strength, high oxidation resistance at high temperatures and optical functionalities [1]. As a result, it has become a ubiquitous material for the fabrication of van der Waals heterostructures [2]. Like many Group III nitride materials, its covalent bonds are highly polar, presenting the possibility of piezoelectric and spontaneous polarizations in the correct crystal configurations. In this talk, I first describe the observation of in-plane piezoelectricity for monolayer (one atom thick) hBN [3], a property that does not exist for bilayer or bulk systems. Next, I report the occurrence of spontaneous out-of-plane polarization and ferroelectricity at anomalously stacked hBN interfaces [4]. We have observed these effects using atomic force microscopy (AFM) electrical modes, namely electrostatic (EFM) and Kelvin Probe (KPFM) Force Microscopy, in combination with detailed modelling of in-plane deformation profiles and interface relaxation. Both the in-plane piezoelectricity and out-of-plane ferroelectricity presented here open up interesting possibilities for precise control of device properties. The experimental approach used here also shows a way to investigate the polarization properties of other materials at the nanoscale.

References

- [1] Li, L. H., Cervenka, J., Watanabe, K., Taniguchi, T., Chen, Y., *ACS Nano* **8**, 1457 (2014).
- [2] Dean, C. R., Young, A. F., *et al.*, *Nat. Nanotechnol.*, **5**, 722 (2010).
- [3] Ares, P. Cea, T., Holwill, M. J., *et al.*, *Adv. Mater.* **32**, 1905504 (2020).
- [4] Woods, C. R., Ares, P., Nevison-Andrews, H. *et al.*, *Nat. Commun.* **12**, 347 (2021).

Figures

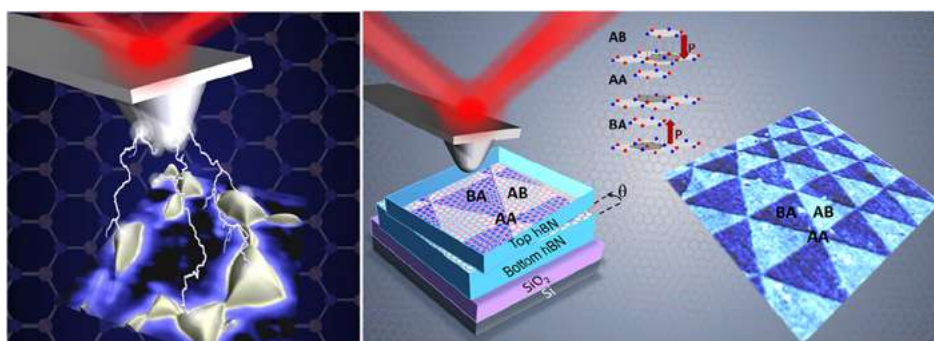


Figure 1: Piezoelectricity and ferroelectricity in hBN.

Magnetic Kondo lattices in two-dimensional transition metal dichalcogenides

Fernando de Juan

Wen Wan, Rishav Harsh, Antonella Meninno, Paul Dreher, Sandra Sajan, Ion Errea, Fernando de Juan, Miguel Ugeda
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Metallic dichalcogenides like 1T-TaSe₂ present an uncommon charge density wave state which produces an array of isolated, unpaired electrons that form a lattice of magnetic moments. In this talk, I will present both theory and experimental results on the 1T/1H-TaSe₂ heterostructure, where the magnetic moments in the T layer are coupled to the Fermi surface of the H layer and form a Kondo lattice. Our STM experiments do reveal a Kondo peak which is however split at very low temperatures. I will then discuss how this splitting and its dependence on magnetic field are not consistent with a Kondo screened, paramagnetic lattice, and rather point to a magnetic ground state with small Kondo exchange. I will then present ab-initio calculations to estimate the Kondo coupling and discuss our results in terms of an Anderson model. Our work uncovers these dichalcogenides as a natural platform to study Kondo lattices [1].

References

[1] Wan et al, arxiv:2207.00096

Figures

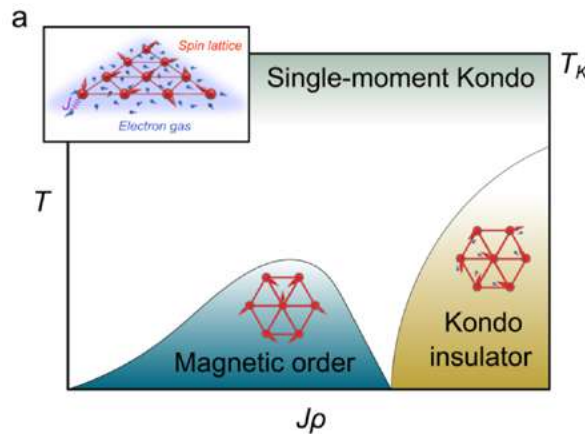


Figure 1: Schematic Doniach diagram showing the competition between magnetic and Kondo screened phases. The inset shows the effective triangular Kondo lattice realized in transition metal dichalcogenide heterostructures.

Universal moiré nematic phase in twisted graphene

Carmen Rubio-Verdú¹

Simon Turkel¹, Yuan Song¹, Lennart Klebl², Rhine Samajdar³, Mathias S. Scheurer^{3,4}, Jörn F. Venderbos^{5,6}, Kenji Watanabe⁷, Takashi Taniguchi⁸, Héctor Ochoa¹, Lede Xian^{9,10}, Dante M. Kennes^{2,9}, Rafael M. Fernandes¹¹, Ángel Rubio^{9,12,13}, Abhay N. Pasupathy¹

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Graphene moiré superlattices display electronic flat bands. At integer fillings of these flat bands, insulating states due to strong electron–electron interactions are generally observed. However, the presence of other correlation-driven phases in twisted graphitic systems at non-integer fillings is unclear. We report [1] the existence of three-fold rotational (C_3) symmetry breaking in twisted double bilayer graphene. Using spectroscopic imaging over large and uniform areas to characterize the direction and degree of C_3 symmetry breaking, we find it to be prominent only at energies corresponding to the flat bands and nearly absent in the remote bands. We demonstrate that the magnitude of the rotational symmetry breaking does not depend on the degree of the heterostrain or the displacement field, being instead a manifestation of an interaction-driven electronic nematic phase. We show that the nematic phase is a primary order that arises from the normal metal state over a wide range of doping away from charge neutrality. Our modelling suggests that the nematic instability is not associated with the local scale of the graphene lattice, but is an emergent phenomenon at the scale of the moiré lattice. This suggest that nematic instabilities are common in moiré systems and may be universal elements of their phase diagrams.

References

[1] Rubio-Verdú *et al.*, *Nature Physics*, **18**, 196 (2022).

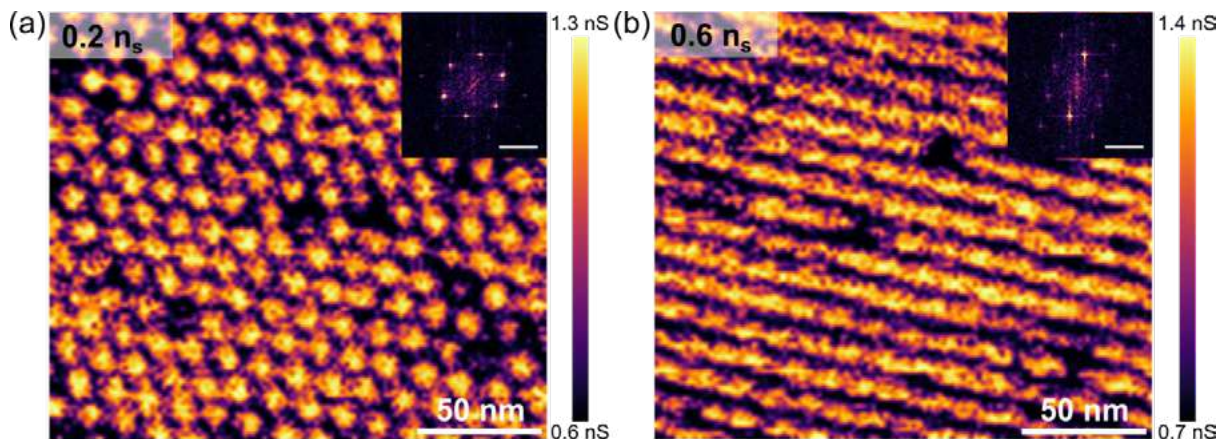


Figure 1: (a), (b), dI/dV maps at the energy of the VFB, close to charge neutrality (a) and around half-filling of the CFB (b). The insets show the fast Fourier transform of each LDOS map.

Graphene field effect transistors for THz technology and applications

Juan Antonio Delgado Notario

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Terahertz (THz) frequency range is still known as one of the least exploited and investigated ranges of the electromagnetic spectrum. Located between the millimeter waves and infrared domain has hazy defined range from about 100 GHz up to 10 THz. THz waves have revealed a great potential for use in various fields and for a wide range of challenging applications such as security, material sensing, future 6G wireless or quantum communication among others. To this aim, high-performance detectors are, vital for exploitation of THz technology. Thus, on the last years, there was a huge scientific interest for the development of new THz devices and techniques. A very special attention has been given to graphene plasmonic THz detectors as they have started to emerge as a promising platform for a new generation of optoelectronic devices, but improving their performance is still necessary. In the lecture we will show how graphene nanostructures forming lateral asymmetric superlattices (Figure 1) can be used for sensitive THz detection operating up to room temperature. Here we will demonstrate that novel approaches and mechanisms could lead to enhance the performance on these graphene-based THz detectors [1]. Furthermore, as a proof of concept two clear examples with these devices will be presented to be used for terahertz sensing of hidden metallic objects at room temperature [2] and as a platform for the experimental observation of the nontrivial topological gap in graphene [3].

References

- [1] J. A. Delgado-Notario et al. Enhanced terahertz detection of multigate graphene nanostructures. *Nanophotonics* 11(3), 519-529 (2022)
- [2] J. A. Delgado-Notario et al. "Asymmetric dual-grating gates graphene FET for detection of terahertz radiations", *APL Photonics* 5, 066102 (2020)
- [3] C. Bray et al. "Temperature-dependent zero-field splittings in graphene", *Phys. Rev. B* 106, 245141 (2022)

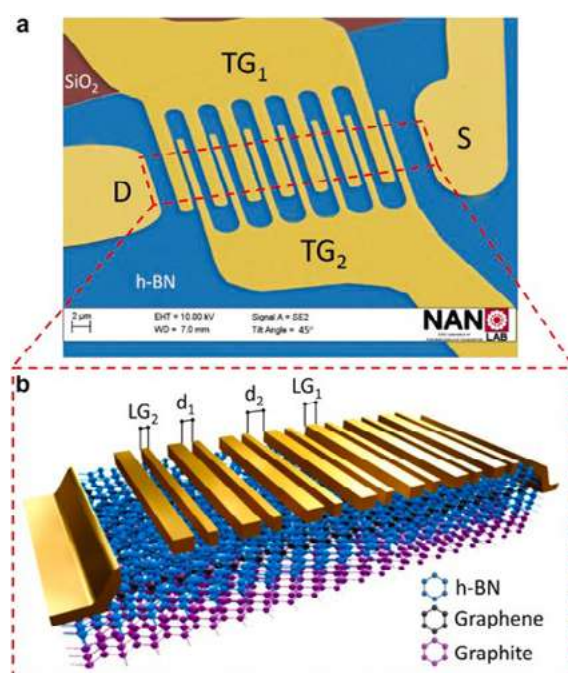


Figure 1: A graphene-based THz detector



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Non-reciprocal charge transport in chiral Tellurium nanowires

Marco Gobbi^{1,2,3}

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Charge-to-spin conversion enables the electrical generation of spin currents without magnets.[1] For instance, the flow of a charge current generates a net spin polarization in materials characterized by strong spin-orbit coupling and broken inversion symmetry through the Edelstein effect. Lacking inversion and mirror symmetry, chiral materials such as elemental Te (Figure 1a) are the ideal playground to explore the relation between structural symmetry and electronic spin transport.[2] Here, we report a chirality-dependent and gate-tuneable charge to spin conversion in single-crystalline Te nanowires.[3] The generation of a net spin polarization is inferred by recording a dependence of the nanowire resistance on the relative orientation between electrical current and applied magnetic field (Figure 1b,c). By analyzing this non-reciprocal charge transport, we show that an electrical current generates a spin polarization oriented along to the chiral axis and pointing in opposite direction for different crystal handedness. Theoretical calculations indicate that this charge-to-spin conversion arises from the radial spin texture of the valence band of Te. In addition, the electric field generated by a gate electrode modulates the amplitude of the non-reciprocal charge transport by a factor six, indicating the possibility to electrically manipulate the efficiency of the charge-to-spin conversion. The all-electrical generation, control, and detection of spin polarization in chiral Te nanowires opens the path to exploit chirality in spintronic devices.

- [1] A. Soumyanarayanan, N. Reyren, A. Fert, and C. Panagopoulos, *Nature* **539**, 509–517 (2016).
- [2] S.-H. Yang, R. Naaman, Y. Paltiel and S. S. Parkin, *Nat. Rev. Phys.*, **3**, 328–343 (2021).
- [3] F. Calavalle, M. Suárez-Rodríguez, B. Martín-García, A. Johansson, D. C. Vaz, H. Yang, I. V. Maznichenko, S. Ostanin, A. Mateo-Alonso, A. Chuvilin, I. Mertig, M. Gobbi, F. Casanova and L. E. Hueso, *Nat. Mater.* **21**, 526–532 (2022).

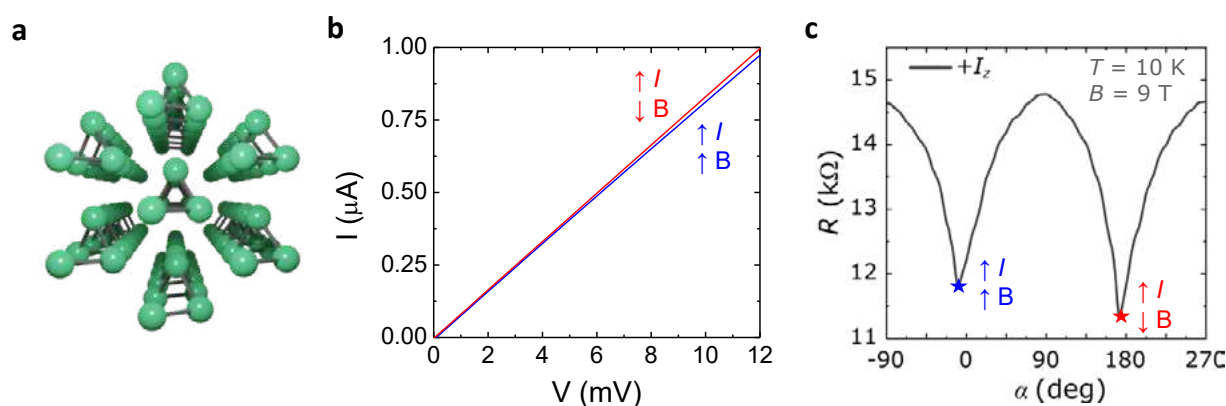


Figure 1: **a.** 3D sketch of the Te crystal structure. **b.** Different current-voltage traces are recorded when the magnetic field is applied parallel or antiparallel to the current, corresponding to different resistance. **c.** Resistance of a Te nanowire as a function of the angle α between the current direction and an external magnetic field.

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

M. R Losada¹

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In this work¹, 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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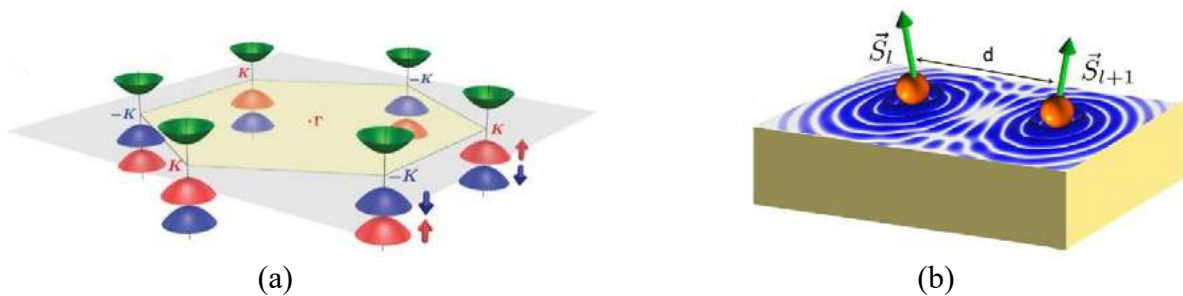


Figure 1: (a) Schematic drawing of the spin-valley coupled band structure (Picture taken from [5]). (b) Scheme of the mechanism of the indirect exchange interaction between two localized surface spins (Taken from [6])

Universality of moiré physics in collapsed chiral carbon nanotubes

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The discovery of superconducting and correlated insulating behavior in twisted bilayer graphene (TBG) has shaken up the field of two-dimensional (2D) materials, reinvigorating the study of graphene-based systems. We demonstrate that one-dimensional moiré patterns, analogous to those found in twisted bilayer graphene, can arise in collapsed chiral carbon nanotubes (CNT) [1]. Performing a detailed study of the electronic structure of all types of chiral nanotubes, previously collapsed via molecular dynamics and validated against ab-initio modeling, we find that magic angle physics occurs in all families of collapsed carbon nanotubes [2]. Velocity reduction, flat bands, and localization in AA regions with diminishing moiré angle are revealed. Remarkably, all kinds of nanotubes behave the same with respect to magic angle tuning, showing a monotonic behavior that gives rise to magic angles in full agreement with those of TBG.

Superconductivity in TBG was an unexpected phenomenon, so the quest for other systems which could be the 1D analogues of TBG is of great importance to elucidate the nature of superconductivity found therein. Moreover, nontrivial topological phases have been found in the magic angle regime and are closely related to flat bands. Therefore, chiral collapsed carbon nanotubes stand out as promising candidates to explore topology and superconductivity in low dimensions, emerging as the one-dimensional analogues of twisted bilayer graphene.

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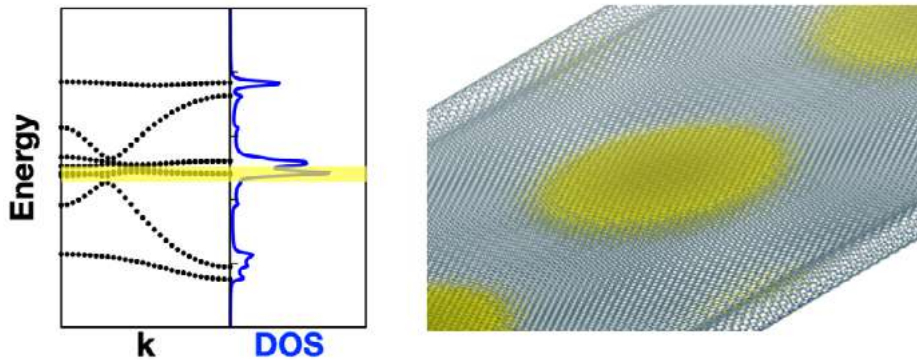


Figure 1: Left panel: Band structure and total DOS for a (164,2) collapsed nanotube. The two highest valence bands are highlighted to indicate the range of energies occupied to map the spatial localization of those states. Right panel: lateral view of the structure with the local DOS of the aforementioned bands highlighted in color. The states are localized in the AA regions of the nanotube unit cell.



When active matter turns solid : from collective motion to collective actuation

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Active matter is made of a large number of out of equilibrium interacting units, which convert some source of energy into directed motion. In contrast with systems driven out of equilibrium by an external field, or through the boundaries, the departure from equilibrium is local and independent for each active unit. Not so surprisingly, active matter exhibits rich collective phenomena at large scales, such as new types of phase separation and/or collective directed motion. The past 25 years have seen a surge of experimental observations and theoretical progress in the description of such phenomena in the realm of active liquids.

There are however a number of circumstances under which the description in terms of liquids is not suited. One can think of ants building solid bridges out of their bodies, meta-materials made of mechanically connected engines, cohesive cell layers or simply very dense assemblies of self propelled particles forming a glass or a crystal. In such cases a description in terms of elastic solid is likely to be more appropriate. However very little is known about the actuation of an elastic lattice by polar active particles, the orientations of which may couple to the displacement field.

In this talk, I will present very recent experimental and theoretical works aiming at developing this new path of research in active matter. Doing so, we shall unveil a new type of collective phenomena, namely collective actuation, and discover how the coupling between linear elasticity and activity leads to a rich selection mechanism of the actuated dynamics.

Rotating vesicles to mimic cell motion

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Cells move through complex media to perform vital biological processes, often following environmental cues. Because the cell membrane is sticky, rather than slipping on surfaces, cells exploit friction to perform controlled motions on surfaces. When two adhering surfaces, the cell membrane and the substrate, are moved across each other, a finite force must be exerted to break the intermolecular bonds across the shearing interface, and these bonds may reform, fully or partially, during sliding. Despite of their importance and complex nature, the tribological properties of cell membranes remain largely unexplored in literature. Therefore, here, we present a minimal cell model to measure and study the tribological properties of cell membranes. The model consists of a vesicle, an aqueous droplet stabilized by an amphiphilic membrane, produced by microfluidics [1], encapsulating a magnetic microparticle in the core, as illustrated in Figure 1. External actuation of the microparticle results in the rotation of the vesicle, which slides on the substrate, enabling tracking of the vesicle motion. Using this approach, we show that rotating vesicles can move exploiting hydrodynamic friction, and that the vesicle velocity can be modified by fine tuning of membrane mechanical properties. Incorporation of protein receptors in the vesicle membrane and specific ligands on the substrate may result in directed motion along gradients in the mechanical properties or ligand concentration in the substrates [2].

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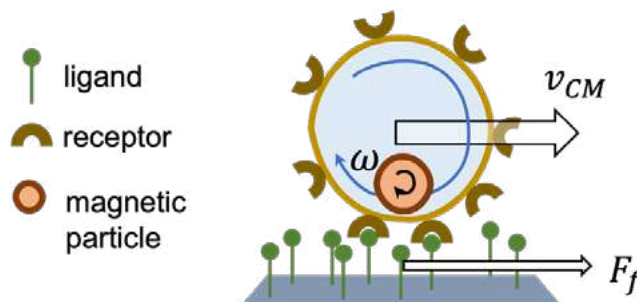


Figure 1: Schematic illustration of a vesicle that rotates upon external actuation of an encapsulated magnetic particle and translates on a substrate with a typical velocity v_{CM} due to a friction force, F_f .

Non-equilibrium active switching of soft colloids: microstructure, phase behaviour and heterogeneous dynamics

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We explore the microstructure and phase behavior of a nonequilibrium system comprised by soft colloids that can actively switch their interactions between two states at a predefined kinetic rate. For this purpose, we employ a Reactive Dynamical Density Functional Theory (R-DDFT) and reactive Brownian-Dynamics simulations (R-BD). We find that the switching rate interpolates between a near-equilibrium binary mixture at low rates and a nonequilibrium monodisperse liquid for large rates, strongly affecting the one-body density profiles, adsorption, and pressure at confining walls. Importantly, we show that sufficiently fast switching impedes the phase separation of an (in equilibrium) unstable liquid, allowing the control of the degree of mixing and condensation and local microstructuring in a cellular confinement by tuning the switching rate [1, 2].

Switching activity also modifies the dynamics and diffusion coefficients of the individual particles, leading to a crossover from short to long times, with a regime for intermediate times showing anomalous diffusion [3]. The corresponding self-intermediate scattering function shows the two-step relaxation patterns typically observed in soft materials with heterogeneous dynamics such as glasses and gels. R-DDFT results are in excellent agreement with R-BD simulations and the analytical predictions of a phenomenological Continuous Time Random theory, thus confirming that R-DDFT constitutes a powerful method to investigate not only the structure and phase behavior, but also the dynamical properties of non-equilibrium active switching colloidal suspensions.

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Nematics in solid tori: Doubly twisted structures and defect populated configurations

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Nematic liquid crystals are partially ordered fluids characterized by an apolar vector field, called director, that represents the average orientation of its anisotropic building blocks. Confining a nematic liquid crystal can frustrate its order, leading to the presence of topological defects, which are regions where the alignment is not defined. Each topological defect can be characterized by a quantity called topological charge. Mathematically, the Poincaré-Hopf index theorem relates the total topological charge to the confining topology. For instance, a 2-sphere must have a total topological charge of +2, so that the presence of defects is mathematically required. In the case of a toroidal surface, the total topological charge must be equal to 0, and thus defect free configurations of the material are allowed. In prior experimental work in our group, we filled a solid torus with a nematic liquid crystal and found spontaneous chiral symmetry breaking without defects [1]. In this talk, we will report on alternative defect-populated configurations [2]. These have $s=\pm 1$ pairs, with the $s=+1$ and $s=-1$ defects most often located in regions of positive and negative Gaussian curvature respectively. Remarkably, we also observe these defect pairs in cylinders. The key is the similar free energy of both defect-free and defect-populated configurations separated by a large free energy barrier.

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Lattice resonances: a collective response of periodic arrays of nanostructures

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Periodic arrays of metallic nanostructures are able to support collective modes known as lattice resonances. These excitations occur at wavelengths commensurate with the periodicity of the array and give rise to very strong and spectrally narrow optical responses. Thanks to these exceptional properties, periodic arrays are being exploited in a wide variety of applications, including ultrasensitive biosensing, nanoscale light emission, and color printing, to cite a few.

In this talk, we will discuss some recent theoretical advances on the topic of lattice resonances. We will pay particular attention to the near- and far-field properties of these modes and how they depend on both the characteristics of the array and the source used to excite them.

Temporal and spatiotemporal metamaterials

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In this talk I will first introduce the basic concepts of wave interactions in time varying media. I will discuss how temporal modulations of the electromagnetic parameters offer new pathways in wave control with metamaterials, as energy is not necessarily conserved in these time-dependent systems, and non-reciprocal effects can be realized [1].

Next, I will concentrate on a class of space-time metamaterials where parameters are modulated in a travelling-wave form, such that there is an apparent motion of the optical properties. Through an homogenization theory that provides analytical expressions for the effective permittivity, permeability and magnetoelectric coupling of these media, I will show how non-reciprocity arises even in the quasistatic limit [2] and how the synthetic motion present in these systems allow us to make a link to the Fresnel drag effect of light in moving media [3]. Additionally I will discuss how an unconventional linear gain mechanism takes place when the modulation travels close to the speed of light [4], resulting in nonreciprocal and broadband amplification that could be realised with graphene [5]. Finally, I will present an implementation of an Archimedes screw for light that leads to chirally-selective amplification [6].

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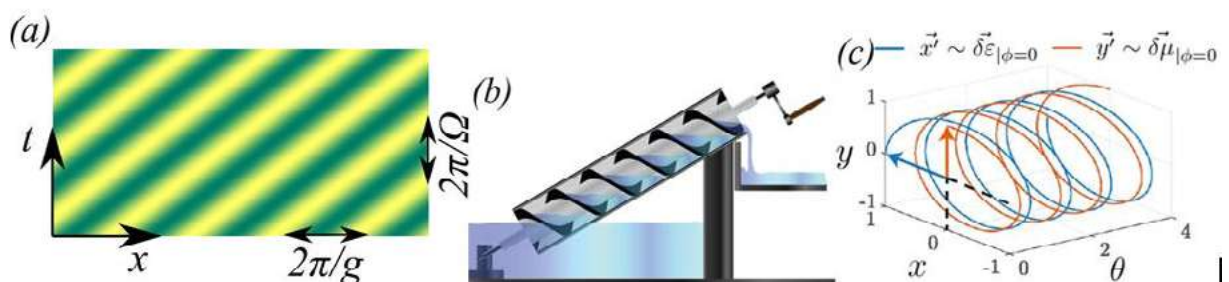


Figure 1: (a) Sketch of space-time modulation of the permittivity and/or permeability of travelling wave kind. (b) A mechanical Archimedes screw carries fluids from a lower to a higher ground. (c) An optical screw is a medium whose permittivity and permeability tensors are modulated such that the principal axes of their modulation describe two helices in the spatio-temporal coordinate.

Fast response photogating in monolayer MoS₂ phototransistor

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Two-dimensional transition metal dichalcogenide (TMD) phototransistors have been the object of intensive research during the last years due to their potential for photodetection. Photoresponse in these devices is typically caused by a combination of two physical mechanisms [1-2]: the photoconductive effect (PCE) and photogating effect (PGE). In earlier literature for monolayer (1L) MoS₂ phototransistors, PGE is generally attributed to charge trapping by polar molecules adsorbed to the semiconductor channel, giving rise to a very slow photoresponse. Thus, the photoresponse of 1L-MoS₂ phototransistors at high-frequency light modulation is assigned to PCE alone. In this work [4] we investigate the photoresponse of a fully h-BN encapsulated monolayer (1L) MoS₂ phototransistor. In contrast with previous understanding, we identify a rapidly-responding PGE mechanism that becomes the dominant contribution to photoresponse under high-frequency light modulation. Using a theoretical model for the photocarrier dynamics, we fit the illumination power dependence of this PGE and estimate the energy level of the involved traps. The resulting energies are compatible with shallow traps in MoS₂ caused by the presence of sulfur vacancies.

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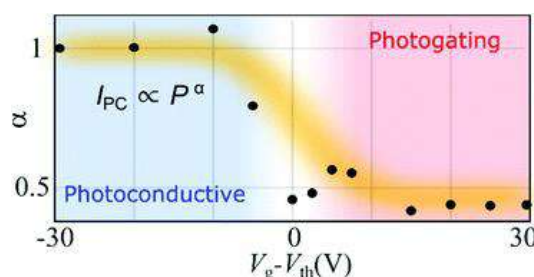
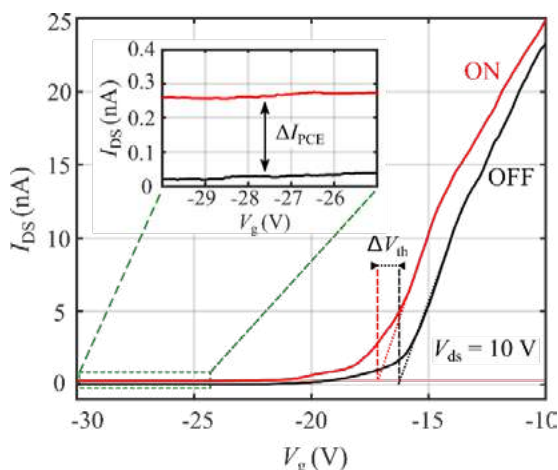


Figure: a) Gate transfer curves of the device, showing a threshold gate voltage $V_{th} = -11$ V. The inset shows a zoom-in of the region indicated by the dashed green rectangle. The contributions to photoresponse by ΔI_{PCE} and ΔI_{PGE} are indicated in the plot. b) Dependence of the fitting parameter α on $V_g - V_{th}$. The two different regimes for power dependence are indicated in the figure

Imaging of Anti-ferroelectric Dark Modes in an Inverted Plasmonic Lattice

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Plasmonic lattice nanostructures are of technological interest because of their capacity to manipulate light below the diffraction limit. Here, we present a detailed study of dark and bright modes in the visible and near-infrared energy regime of an inverted plasmonic honeycomb lattice by a combination of state-of-the-art Au+ focused ion beam lithography, optical and electron spectroscopy, and finite-difference time-domain simulations. The lattice consists of slits carved in an Au thin film, exhibiting a plethora of resonances in the visible and near-infrared ranges.

A detailed description of the charge distribution and near-field enhancement has been given by virtue of the good agreement between the electron energy loss spectroscopy (EELS) measurements, the optical measurements, and simulations. The most remarkable result is the finding of dark modes that may be caused by antiferroelectric arrangements of the slit polarizations, giving rise to charge arrangements with a unit cell four times larger than that of the original honeycomb lattice (see Figure 1(b and 1e)). Additionally, bright plasmonic modes exhibiting hotspots far from the metal slits are also found. The studied plasmonic resonances take place within 0.5 and 2 eV energy range, indicating that they could be suitable for a synergistic coupling with excitons in 2D transition metal dichalcogenides materials or for designing nanoscale sensing platforms based on near-field enhancement over a metallic surface. For example, the exciton energies for 2D WSe₂ and MoS₂ on an Au substrate, 1.75 and 1.9 eV, respectively [1], could be targeted by easily tuning manufacturing parameters such as the pitch of the lattice, thus changing the spectral position of the plasmonic resonances.

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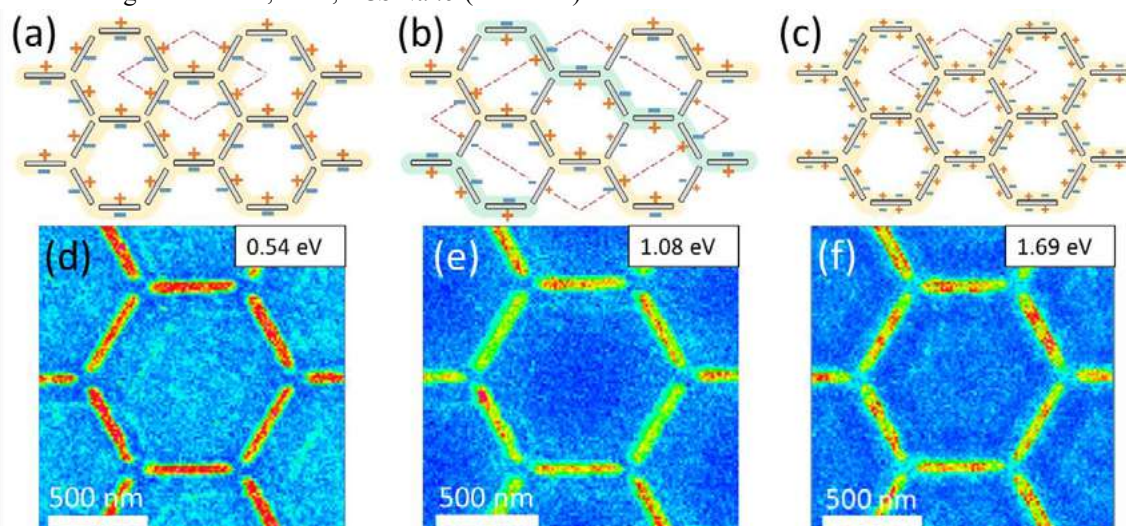


Figure 1. Plasmonic modes measured in the lattice at three different energies. (a), (b) and (c) show schematic representations of the charge distributions associated with one bright and two dark modes, respectively. Panels (d), (e) and (f) present the EELS mapping for the each of the modes depicted in the upper panels.

The emergence research landscape of altermagnetism

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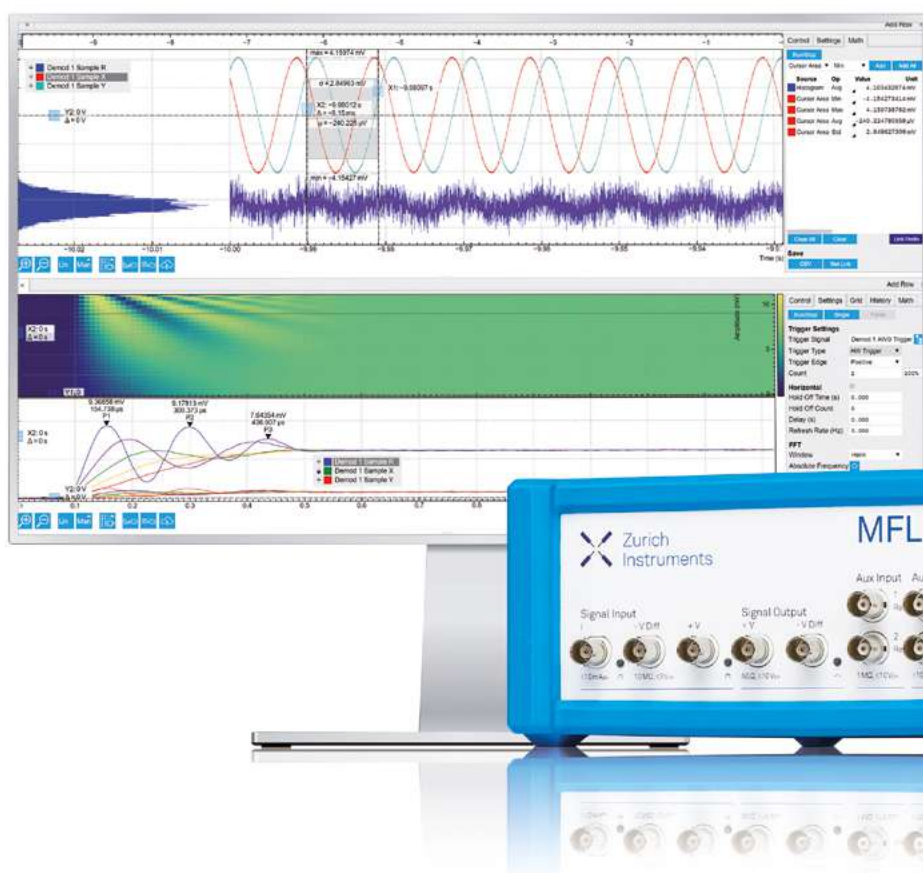
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Antiferromagnetic spintronics has been one of the most active research areas of condensed matter in recent years. As we have learned how to manipulate and understand antiferromagnets actively and their emergent topology, further surprises awaited. Turning off spin-orbit coupling, a new fresh view at the family of antiferromagnetic ordered systems reveals also an emergent new class, dubbed altermagnets, with properties unique to itself and separate from ferromagnets and antiferromagnets. We report the discovery of a third distinct magnetic phase, beyond the conventional ferromagnetism and antiferromagnetism, with non-relativistic alternating spin-momentum locking, which we dub "altermagnetism". We show that this new phase is as abundant in nature as conventional ferromagnetism and antiferromagnetism, while it displays properties unparalleled in the two traditional magnetic phases, such as spin splitting by electric crystal field. Remarkably, altermagnetism was missed over the past century of quantum-magnetism research because it cannot be identified by the conventional crystallographic and relativistic magnetic symmetries, established since the early works of Bethe, Landau, Shubnikov and others. This altermagnetic phase emerges naturally when utilizing the spin-symmetry formalism, where spin and real space are decoupled.

Desafíos.

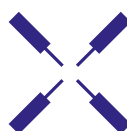
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Direct X-ray detection of the spin Hall effect in CuBi

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The spin Hall effect, and its inverse, are important spin-charge conversion mechanisms widely investigated due to their fundamental importance in the development of spintronics devices. Their measurement is typically done by electrical detection schemes involving an interface with another magnetic material and thus, a combination of the properties of both materials as well as the interface are measured. The large scattering of reported results from these methods for the same material and temperature call out for a more direct and interface-free approach. Optical detection schemes have been successfully used for the determination of SHE in semiconductors. This approach is, however, challenging for metallic systems, due to their considerably shorter spin diffusion lengths. Only recently, optical measurements for Pt and W have been reported [1].

Considering that x-ray magnetic circular dichroism (XMCD) has become a reference tool for precision measurement of small or diluted magnetic signals, we propose the use of XMCD-PEEM microscopy for direct, interface-free determination of SHE in metals. In particular, we report the observation of spin separation due to SHE in a single layer of Bi-doped Cu (Cu₉₅Bi₅), a material in which giant SHE has been reported [2,3]. We performed interface-free x-ray spectroscopy measurements at the Cu L_{3,2} absorption edges while applying electrical current to the sample. The sign of spin accumulation depends on the direction of the current (Figure 1.a) and the amplitude of the X-ray magnetic circular dichroism (XMCD) signal scales with the current density and has different sign when measuring at the L₂ or L₃ absorption edges, as expected for SHE (Figure 1.b). We have measured an induced magnetic moment of $(2.7 \pm 0.5) \times 10^{-12} \mu_B \text{ A}^{-1} \text{ cm}^2$ per Cu atom averaged over the probing depth, which is of the same order as for Pt measured by magneto-optics. Our results constitute the proof of concept for the direct, interface free and element-selective measurement of the SHE in a single material by means of X-ray spectro-microscopy, and highlight the potential of CuBi for spin-charge conversion applications[4].

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All-electrical spin control in low-symmetry materials

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The existence of the quantum spin Hall (QSH) insulator has boosted opportunities for spintronics and quantum metrology, given the ability of topologically protected states to convey spin information over long distances at ultralow dissipation rate. QSH is a manifestation of strong spin-orbit coupling. However, even in time-reversal symmetric systems, the lack of a spin conservation axis in QSH insulators allows backscattering effects for edge states, limiting their ballistic transport. In some situations, the emergence of a phenomenon known as persistent spin texture (PST) enforces spin conservation and favors long spin lifetimes even in the presence chemical disorder and structural imperfections. Such an effect is deeply rooted in the underlying symmetries of the system and opens promising prospects for spintronics when combined with the manifestation of dissipationless chiral edge states. The recent prediction and experimental observations of a PST-driven canted quantum spin Hall effect in low-symmetry monolayer WTe₂ provide new ingredient for the use of topological materials in spintronic applications.

This work reports on the possibility of a fully controllable variation of up to 90 degrees rotation of the spin polarization of chiral edge-states, dictating the canted QSH effect, while preserving spin conservation. By combining density functional theory (DFT) with tight-binding methods and quantum transport simulations, we show that the emerging PST can be continuously varied from in-plane to out-of-plane under electric fields below 0.1 V/nm, making this effect experimentally accessible. The experimental confirmation of such fully electrically tunable spin-polarized topological currents would establish a new milestone towards replacing magnetic components in spintronic devices and all-electric spin circuit architectures, as well as optimized resistance quantum standards.

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Coexistence of structural and magnetic phases in van der Waals magnet CrI_3

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Amidst the members of the family of layered materials, chromium triiodide (CrI_3) was the first one to demonstrate the persistence of a ferromagnetic hysteresis down to the monolayer as well as a layer-dependent transition from a ferromagnetic to an antiferromagnetic state [1]. Following this discovery, a plethora of studies appeared providing evidence that the origin of this thickness-dependent magnetism relies in the crystalline stacking order, thus revealing a strong coupling between magnetism and crystal structure [2,3,4]. However, to date, bulk CrI_3 keeps hosting fundamental conundrums such as the emergence of a peak at 50 K in the in-plane magnetization curve, and controversies, such as having a range of temperatures for the crystalline phase transition [4,5]. Combining muon spin rotation, magnetization and low temperature X-ray diffraction measurements (Figure 1) we reveal the emergence of two unexpected magnetic phases as well as the persistence of 10 % of the monoclinic phase at low temperature. These two events give hints of a rich phase diagram regarding 2D magnetism in CrI_3 , which goes far beyond the assumed monoclinic/rhombohedral dichotomy.

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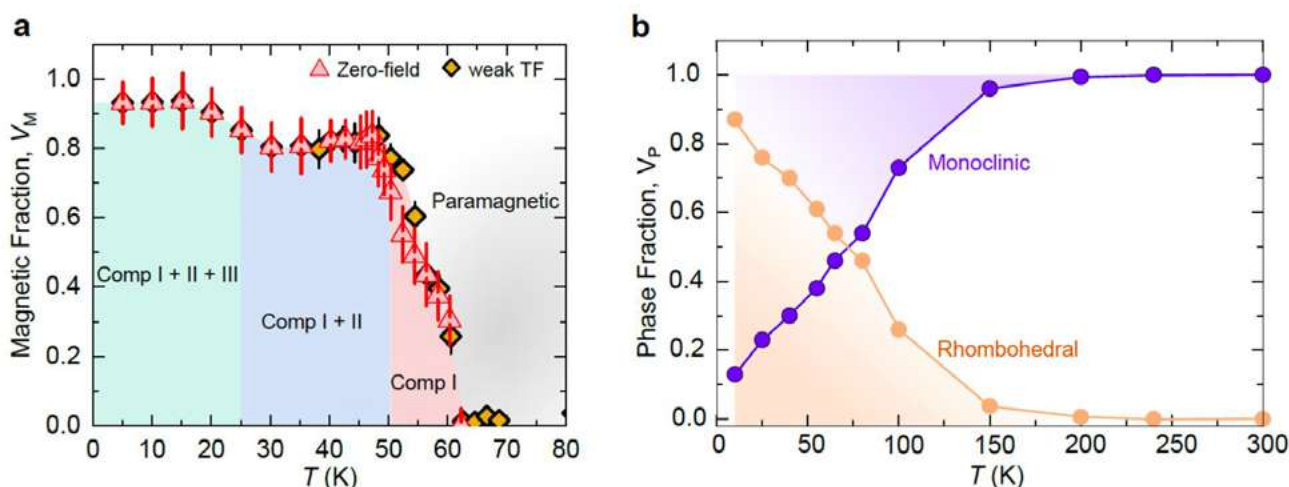


Figure 1: **a**, Temperature dependence of the total magnetic volume fraction V_M determined by zero field μSR measurements. **b**, Crystalline phase fraction obtained from Rietveld refinements on temperature dependent X-ray diffraction measurements.

Lightwave Control for Sub-Cycle and Non-Resonant Valley Manipulation in 2D Materials

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Modern light generation technology offers extraordinary capabilities for sculpting light pulses, with full control over individual electric field oscillations within each laser cycle [1]. These capabilities are at the core of lightwave electronics on a few-cycle to sub-cycle timescale, aiming at information processing at peta-Hertz rates. At the same time, quantum materials encompass fascinating properties such as the possibility to harness extra electronic degrees of freedom, e.g., the valley pseudospin, that can be optically initialized via resonant circular pulses [2,3,4]. Still, initializing, manipulating and reading the valley degree of freedom on timescales shorter than valley depolarization remains a crucial challenge.

I will present an all-optical, non-resonant approach to control the injection of carriers into the valleys by controlling the sub-cycle structure of non-resonant driving fields [5]. For triangular sub-lattices, such as those of hexagonal boron nitride (hBN) or MoS₂, the bicircular field, formed by a circular field and its counter-rotating second harmonic, possesses the symmetry of the sub-lattice and is shown to initialize a high degree of valley polarization on a sub-cycle timescale. The valley pseudospin is then read by using either the imprint of the Berry curvature on the high harmonic generation spectrum in non-inversion-symmetric monolayers [5] or by quantifying the appearance of even harmonics due to the breaking of inversion symmetry created by the valley polarization [6].

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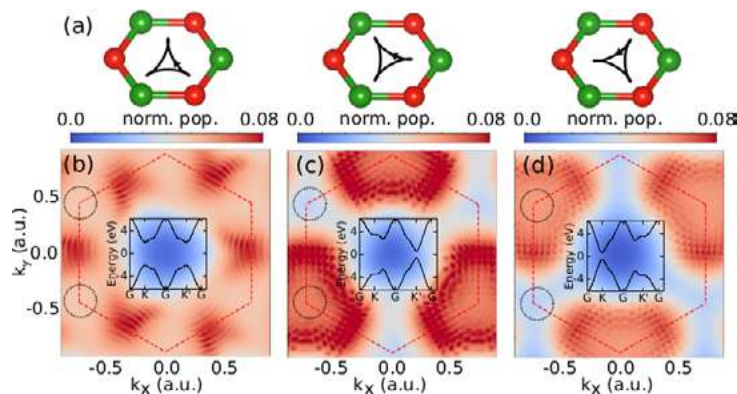


Figure 1: (a) Different orientations of the bicircular field with respect to the lattice, controlled by the phase delay between the two colors. (b-d) Normalized electron population in the lowest conduction band of hBN after applying the bicircular field above with 3 micron of fundamental wavelength.

Optical bistability based on the integration of a molecular nanomaterial in Silicon Photonics

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Electro-optical bistability is a functionality which can be crucial for a wide range of applications as it can enable non-volatile and ultra-low power switching performance [1]. In this work an advance in Nanophotonics is presented with a new approach for the development of low-power on-chip optical switching devices. This new approach is based on the integration of an encapsulated molecular nanomaterial that presents bistable Spin Crossover (SCO) phenomenon near room temperature (RT) in the Si platform [2].

SCO is a spin-state switching phenomenon present in some molecular compounds such as the coordination complexes of transition-metal ions in which, under certain external stimulus (variation of temperature, pressure, electric field, or light irradiation), the electronic configuration can be switched between two molecular spin states, Low Spin (LS) and High Spin (HS) states [3]. Furthermore, the spin state change is accompanied by a change in the structural, magnetic, and optical properties, as well as in the electrical conductivity and color. These properties vary as a function of the external stimulus following a hysteretic response, recognized as one of the most promising aspects of the system since hysteresis confers bistability and thus a memory effect (Figure 1a).

Finally, the SCO material can be synthesized as nanoparticles so that it can be easily integrated in the silicon platform and have the potential to allow optical switching at room temperature (Figure 1b).

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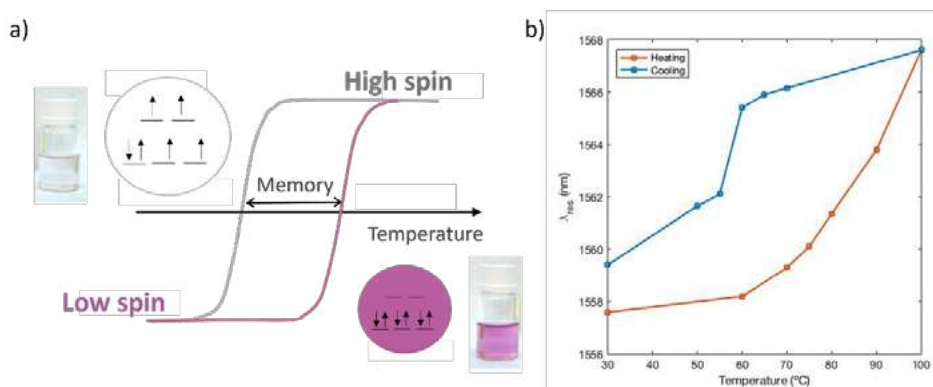


Figure 1: (a) Schematic of the spin configurations and typical spin transition curve with abrupt hysteresis. In the low spin state (LS), electrons are paired, the color of the complex is purple/pink, and the volume is smaller. In the high spin state (HS), the electrons are unpaired, the complex gets a transparent color and the volume increases. (b) Measurement of the optical signal (λ_{res} , resonance frequency) as a function of the temperature where the expected hysterical response is clearly observed.

Periodically driven chiral engine beyond the Carnot limit

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Classically, the power generated by an ideal thermal machine cannot be larger than the Carnot limit. This profound result is rooted in the second law of thermodynamics. Whether this bound is still valid for microengines operating far from equilibrium is an open question in quantum thermodynamics. Here, we demonstrate [1] that a quantum chiral conductor driven by AC voltage can indeed work with efficiencies much larger than the Carnot bound. Our pump engine [see Fig. 1(a)] consists of a scatterer of arbitrary energy-dependent transmission tunnel coupled to electronic hot and cold reservoirs in the presence of an external AC bias voltage. An AC driving typically generates a finite input power that diminishes the efficiency. Our key idea to overcome this difficulty is to selectively apply an AC external field to the electrons depending on the direction, which can be implemented using a chiral conductor such as those created in two-dimensional systems (topological or quantum Hall conductors) [see Fig. 1(b)]. This completely avoids any AC input power, allowing a high efficiency of the quantum engine, in contrast to nonchiral cases. Nonetheless, entropy production is always positive when using the proper definition for AC driven conductors beyond weak coupling [2] and the second law is preserved. The role of the AC driving can be interpreted as a nonequilibrium demon [3] as the driving induces additional entropy production by rearranging the electron energy distribution in a more uncertain way, while injecting zero net energy. Our results are relevant in view of recent developments that use small conductors to test the fundamental limits of thermodynamic engines.

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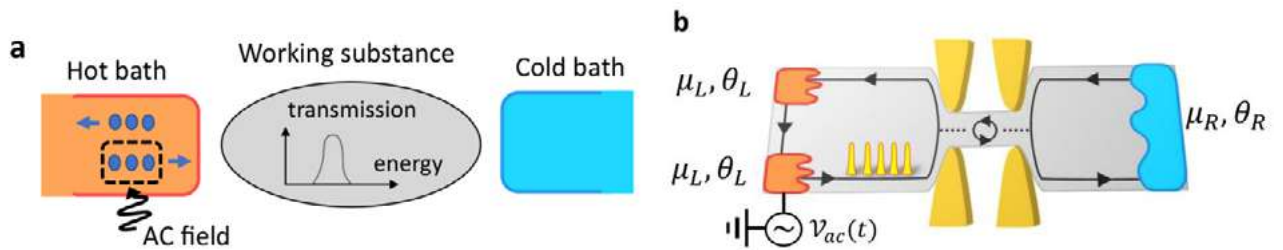


Figure 1: (a) Schematic of periodically driven chiral engine. (b) An implementation using a chiral conductor. $\mu_{L(R)}$ and $\theta_{L(R)}$ are chemical potential and temperature of left (right) reservoir.

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

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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 $\lambda_p/4.5=\lambda_0/50$ (λ_p is the polariton wavelength and λ_0 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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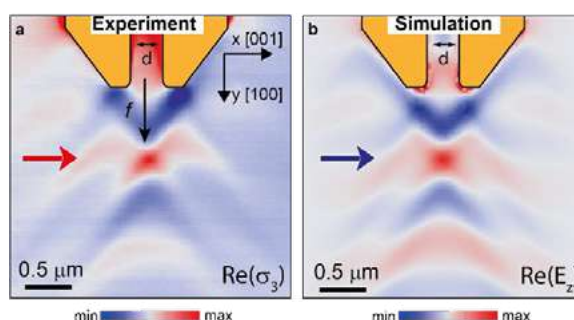
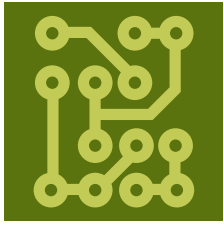


Fig. 1 Nanofocusing of PhPs along the surface of a α -MoO₃ flake into deep-subwavelength focal spots.



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Message from the Editor-in-Chief

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Layered hybrid metal-halide perovskites under strain: insights from photoluminescence and micro-Raman spectroscopy

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Layered hybrid organic-inorganic metal halide perovskites (HOIPs) have emerged as promising materials for optoelectronic device applications, namely due to their tunable bandgap and high carrier mobility. For the successful integration of these materials into devices it is key to understand the relationship between composition, crystal structure and optical properties and how to control them.[1] In particular, research has been directed toward the modulation of their optical properties, with special attention on their photoluminescence (PL). Therefore, several strategies have been proposed such as the variation of their organic-inorganic composition[1], or the application of strain[2,3]. Indeed, strain engineering has demonstrated to be an effective strategy to modulate the optoelectronic properties of 2D materials.[4] However, it has been barely explored on HOIPs. Here, we report the tuning of the micro-photoluminescence emission of 2D lead-bromide HOIP flakes subject to biaxial strain. To generate the mechanical strain, we placed the flakes by viscoelastic stamping on a rigid SiO₂ ring platform, leading to the formation of domes (Figure 1a). At low temperatures, we found that a strain < 1% can change the PL emission spectrum from a single peak (unstrained) to three well-resolved peaks (Figure 1b). Combining temperature-dependent micro-PL and Raman spectroscopy mapping (Figure 1c) and reverse mechanical engineering strain modeling, we confirm that the emergence of the two new PL peaks is related to tensile and compressive thermo-mechanically generated strain coexisting along the flake surface and thickness.[5] Our findings provide new insight into strain-based optoelectronic and sensing devices using 2D HOIPs, leveraging on the design of material composition and substrate platform design.

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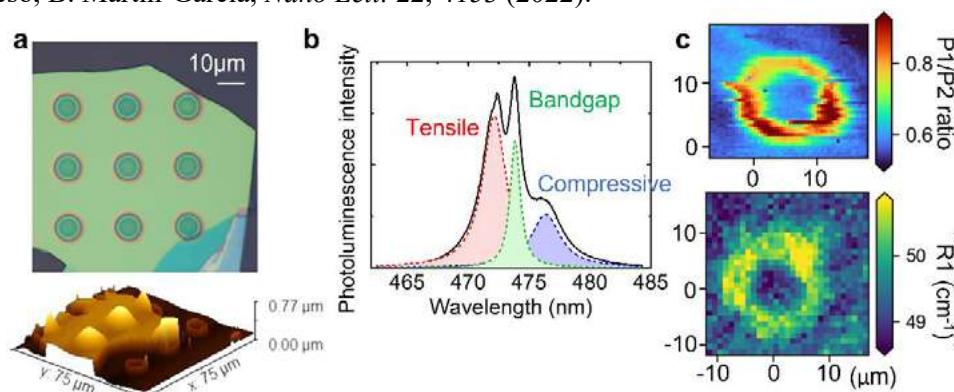


Figure 1: **a**, Optical microscope image of the flake placed on the rings accompanied by a topography reconstruction of two domes. **b**, Representative photoluminescence emission in the regions close to the ring. **c**, low-temperature photoluminescence and Raman mapping of a dome.

Fundamentals and applications of the voltage-triggered insulator to metal transition

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Many correlated oxides feature an insulator to metal transition (IMT) with a large change of resistivity. Generally, these transitions can also be induced electrically, a phenomenon known as voltage-triggered IMT [1,2]. The associated volatile resistive switching has attracted a lot of attention due to potential applications in optoelectronics, neuromorphic computing or rf switches [3]. Despite the wide interest, the fundamental aspects of this voltage-triggered IMT are not well understood. In this talk I will discuss the underlying physics of this phenomenon [1], including topics such as what governs the characteristic length- and time-scales [2,4].

I will also review the current efforts towards applications, with an emphasis on neuromorphic [3,5,6] and probabilistic computing [7].

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New electrocaloric oxides for sustainable and efficient refrigeration

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As refrigeration is essential for health and comfort, food, medicine or electronics, it represents a large and growing fraction of the worldwide electricity consumption. The current cooling technology, based on the compression of harmful gases, has a limited energy efficiency and contributes significantly to global warming. Caloric effects are among the most promising climate-friendly alternatives because they lead to higher energy efficiencies and use solid refrigerants that can be prepared without toxic elements. Electrocaloric (EC) materials show reversible thermal changes when subjected to variations of an applied electric (E) field, known as the electrocaloric effect (ECE), which maximizes near a ferroelectric phase transition [1]. While the research in their magnetocaloric (MC) counterparts is rather mature, EC materials have been in the spotlight only in the last ten years [2], being advantageous over MC because of the ease of application of E fields. Up to now, the research in EC materials has been dominated by lead-based oxides. Sufficiently large ECE values for cooling applications have only been observed in thin-film samples.

We have investigated new EC oxides (bulk and thin film) by making use of in-house laboratory methods for the “direct” and “indirect” measurements of the ECE, combined with complementary synchrotron-based X-ray absorption spectroscopy. In particular, layer-structured ferroelectric Aurivillius oxides $\text{Sr}_{n-3}\text{Bi}_4\text{Ti}_n\text{O}_{3n+3}$ ($n = 4, 5$), where the A- and B-site of the “n” perovskite-like layers are occupied by Sr/Bi and Ti, respectively. The Curie temperature T_C of their ferroelectric transitions is about 800 K and 560 K for $n = 4$ and 5, respectively. Aiming at enhancing their EC response at near room temperature (RT), chemical substitutions at the A- (La^{3+}) and B-site (Nb^{5+}) have been applied to tune T_C close to RT. For both series of compounds ($n = 4, 5$), we found that La-doping is effective in decreasing T_C and in promoting a relaxor ferroelectric behavior but at the expense of weakening the ferroelectricity and EC properties. Preliminary results (Fig. 1) for $\text{Sr}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ ($n=5$) show a promising direction towards enhancement of the EC properties through a combination of La- and Nb-doping featuring an ECE maximum close to RT [3].

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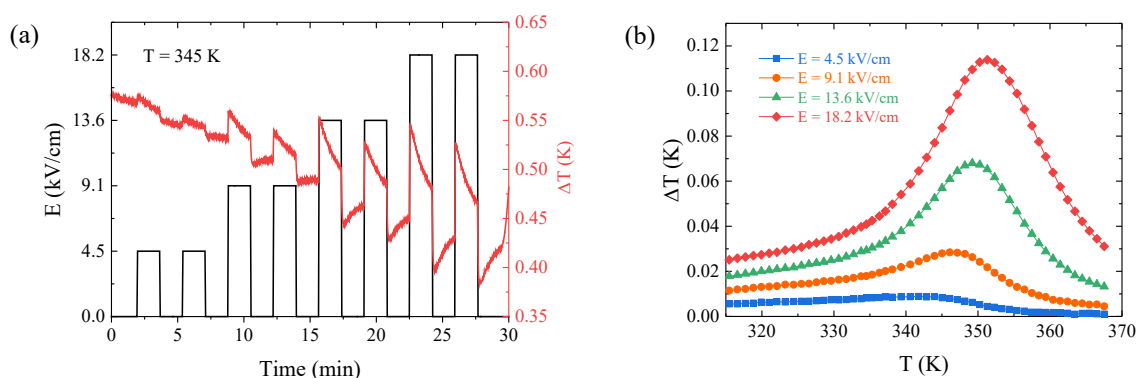


Figure 1. Direct measurements of the ECE temperature change (ΔT), obtained with a quasi-adiabatic calorimeter, for $\text{Sr}_2\text{Bi}_{3.44}\text{La}_{0.5}\text{Ti}_{4.8}\text{Nb}_{0.2}\text{O}_{18}$ at several applied field values. (a) Example of a measurement at $T = 345$ K as a function of time, and (b) ΔT values as a function of temperature, measured upon heating.

Combining Freestanding Ferroelectric Perovskite Oxides with Two-Dimensional Semiconductors for High Performance Transistors

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Field Effect Transistors (FETs) based on silicon technology are facing limits during the last years. To overcome this obstacle an approach to miniaturize even more the devices can be developed, besides the performance can be improved to lower the power consumption, and thus the heat dissipation. But another approach can be used, which consists of adding new degrees of freedom, such as the polarization in a ferroelectric material, hence the device functionality is increased.

The remarkable properties of 2D materials together with their reduced vertical dimensions, directly positioned them as potential components in FET fabrication [1]. The extensive work, particularly on transition metal dichalcogenides-based FETs have proven their suitability, even surpassing the typical characteristics of the silicon-based transistors [2]. Moreover, the recent development of strategies to isolate complex oxide layers and manipulate them similarly to their van der Waals counterparts has placed new tokens on the board [3,4].

In this work [5], we integrate freestanding single-crystalline BaTiO₃ with monolayer MoS₂ flakes, showing mobilities larger than the ones obtained with standard SiO₂ and in the same order of magnitude of devices built with hexagonal boron nitride, which has already shown outstanding electrical properties in FETs [6]. Besides, the devices made with BaTiO₃ show a wide hysteresis related to ferroelectric polarization switching in their electrical transfer curves, an appealing property in memory storage devices.

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Extremely long-range, high-temperature Josephson coupling across a half-metallic ferromagnet

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The Josephson effect results from the coupling of two superconductors across a non-superconducting spacer to yield a quantum coherent state. In ferromagnets, singlet (opposite-spin) Cooper pairs decay over very short distances, and thus Josephson coupling requires a nanometric spacer. In systems with particular properties, however, equal spin triplet Cooper pairs can be generated, allowing the coupling of superconductors across magnetic barriers over much longer distances. Despite many experimental hints of triplet superconductivity at ferromagnet/superconductor interfaces, long range triplet Josephson effects across ferromagnetic barriers have remained elusive. We demonstrate extremely long range high-temperature Josephson coupling across the half-metallic manganite $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ combined with the superconducting cuprate $\text{YBa}_2\text{Cu}_3\text{O}_7$. This is shown in planar junctions which display the hallmarks of Josephson physics: critical current oscillations (Fraunhofer pattern) and quantum phase locking under microwave excitation (Shapiro steps). Interestingly, both in the Fraunhofer pattern and in the Shapiro steps, a strong second harmonic can be observed, which further confirms the exotic superconducting state that can be present in this system. [1-3] The marriage of high-temperature quantum coherent transport and full spin polarization brings unique opportunities for the practical realization of superconducting spintronics, and enables novel strategies for devices in quantum technologies.

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Probing and tuning the electronic properties of low dimensional van der Waals materials

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Probing and tuning the electronic transport properties of low dimensional van der Waals (vdW) materials may represent one of the routes that can satisfy the requirements of modern electronics advancements. The low dimensionality of such materials is not only of interest for scalability purposes in electronic applications, but it brings into the game new and exotic physical phenomena, which can also be tailored creating artificial systems with on demand properties, the so-called vdW heterostructures. Following these two ideas, in one part of my thesis, I studied the interplay between the chirality of the Te nanowires, its band structure, and the charge-to-spin interconversion phenomena occurring when electrical current is applied to this low symmetrical structure [1]. The other part of the work, which is presented here, focused on the molecular tuning of vdW materials' properties. We employed hybrid organic/inorganic heterostructures with the idea of exploiting the chemical flexibility of molecular compounds, to obtain functions by design.

In particular, in the first work (Fig. 1 a)) we tailored the superconductivity of single layer NbSe₂ via self-assembled molecular adlayers. A programmable modulation of the superconducting critical temperature (T_C) was achieved through carrier density variations induced by strong dipolar interaction developing between NbSe₂ and the self-assembled molecular layer [2].

In the second work (Fig. 1 b)), we demonstrate the emergence of a spinterface effect at the interface between prototypical layered magnetic metal Fe₃GeTe₂ and thin films of Co-phthalocyanine. Magnetotransport measurements show that the unpaired spins in Co-phthalocyanine develop antiferromagnetic ordering that pin the magnetization reversal of Fe₃GeTe₂ [3]. In both works the modulation of T_C and the exchange bias induced by the molecules is competitive with the results reported by previous studies trying other approaches, demonstrating the potential of molecular functionalization to tailor the properties of vdW materials.

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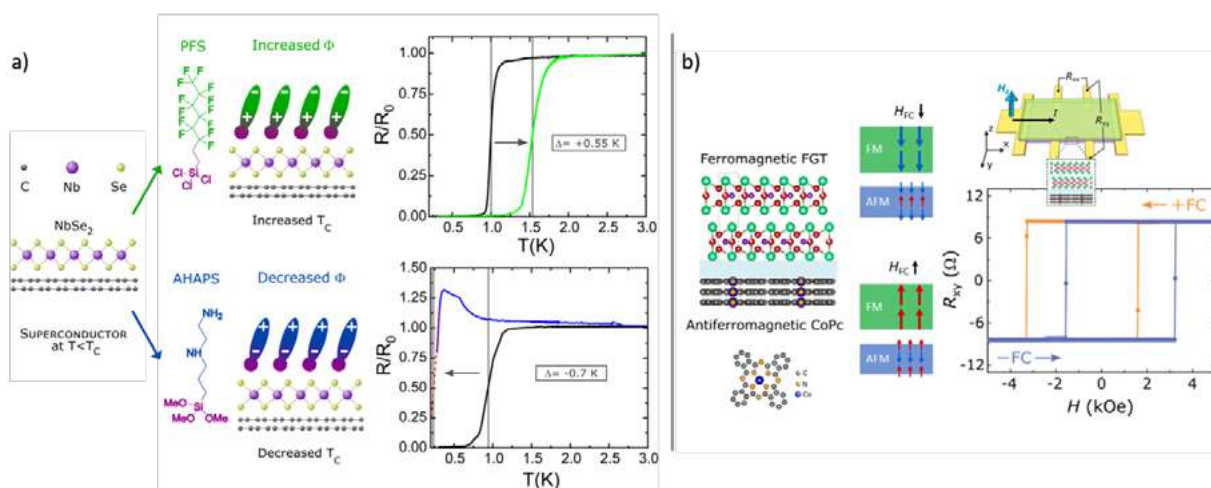


Figure 1: a) Superconductivity modulation in large-area single-layer NbSe₂ via self-assembled molecular adlayers. b) Exchange bias in CoPc/Fe₃GeTe₂ van der Waals heterostructure induced by a spinterface effects.

Topological Materials from a Symmetry Perspective

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In this talk I will be presenting the main results of my thesis, mainly the 3 most relevant papers. First, our work on PbTe, a rock-salt structure material that can present a topological transition as a function of hydrostatic pressure. Second, the ferromagnetic pyrite CoS₂, a well-studied material that we analyze from the topological perspective, finding nodal lines and Weyl nodes with their respective surface states. Lastly, we explore the role of symmetry in time-dependent elastic deformations of a topological semimetal, which gives rise to a new, purely 3-dimensional hydrodynamic response known as hall viscosity.

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Figures

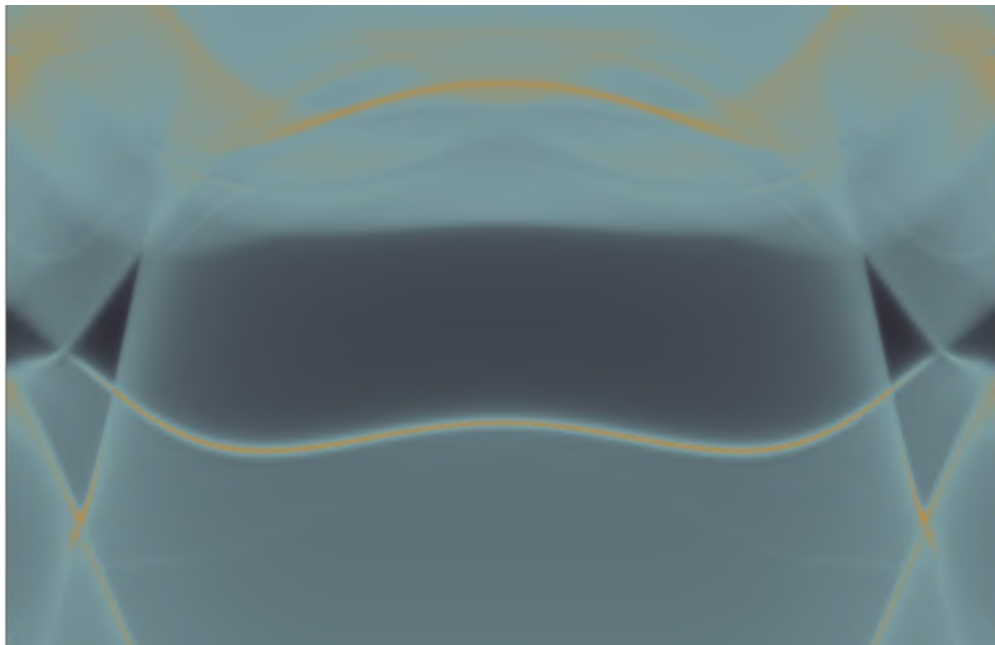


Figure 1: Fermi arcs connecting the projection of Weyl nodes in the (100) surface.

On symmetry and topological aspects of novel phases of matter

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This thesis addresses three classes of topological phases of matter: topological insulators, nodal semimetals and $\mathbb{Z}_2$ topologically ordered states. Their distinctive properties are analyzed combining condensed matter and high energy techniques that depart from their low-energy quasiparticles and their symmetries.

A salient feature of topological insulators is the existence of quantized observables in terms of fundamental constants. By means of effective field theory and tight-binding modeling, we demonstrate that the quantization of circular dichroism in chiral higher-order topological insulators is possible by choosing suitable frequency windows for light absorption.

Nodal semimetals also manifest quantization through the circular photogalvanic effect. We characterize this optical response for the material CoSi by means of a $\mathbf{k} \cdot \mathbf{p}$ analysis to scrutinize its recent experimental observation. These systems are generally described at low energies by small Bloch Hamiltonians; we additionally develop a group theory method to determine any physical observable associated with these finite Hamiltonians without the explicit use of its eigenstates, which allows to avoid unnecessary complications coming from their phase arbitrariness. Finally, we apply renormalization group theory in Weyl semimetals to analyze the emergence of symmetries at low energies under the influence of Coulomb interactions.

In general, intrinsic topological order comes hand in hand with strong correlations that challenge its microscopic study. By exploiting local and global symmetries, we construct ideal models that analytically capture the universal properties of systems with a finite density of $\mathbb{Z}_2$ anyons, conforming whether a Fermi liquid or a Bose-Einstein condensate.

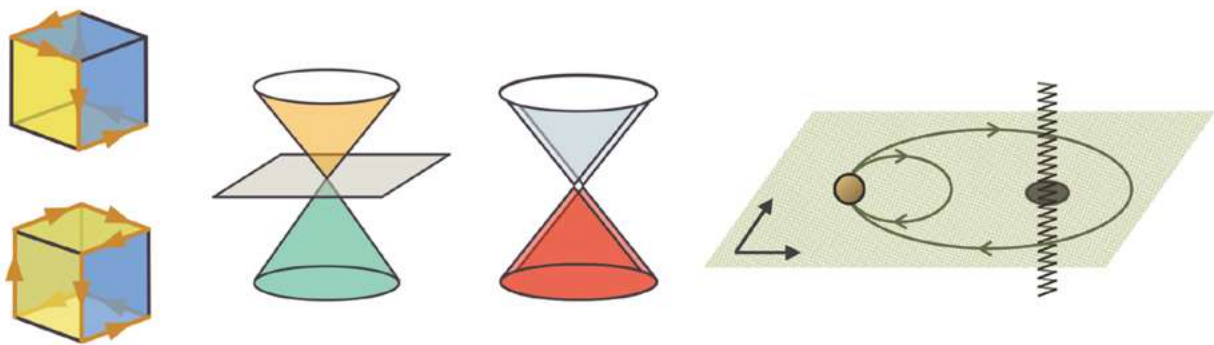


Figure 1: Illustration of the topological phases of matter considered in this thesis.

Quantum devices for thermodynamics at the nanoscale

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As we miniaturize devices to reach the quantum regime, the needs arises to test the laws of thermodynamics in a new realm, in which fluctuations and quantum effects play a very important role. I will discuss how to explore the thermodynamics of the semiconductor devices at nanometer scales, and I will show how we measure the thermodynamic cost of recording the passage of time. We find that the accuracy of our clock and the entropy produced by it are proportional, as predicted both for classical and quantum regimes.

Coupling charge or spin states to mechanical motion might allow us not only to build nanoscale motors but to measure the thermodynamic cost of quantum information processing. Fully suspended carbon nanotube devices allow us to control mechanical, electronic and spin degrees of freedom with high accuracy. Using these devices we find that the coupling of electron transport to the nanotube displacement is ultra-strong. I will discuss how this experimental platform can allow for the study of non-chip quantum energetics.

Visualizing waves and quantum well states at the surface of the heavy Fermion URu₂Si₂.

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Electrons can form a two-dimensional electron gas at metal surfaces, where lateral confinement leads to quantum-well states. Such states have been observed for highly itinerant electrons but remain challenging to visualize in strongly correlated systems because correlations often reduce the separation between energy levels. Here we use millikelvin scanning tunneling spectroscopy to study atomically flat terraces on U-terminated surfaces of the heavy-fermion superconductor URu₂Si₂ which exhibits a mysterious hidden-order state below 17.5 K. We observe two-dimensional heavy fermions (2DHF) made of 5f electrons with an effective mass 17 times the free electron mass. The 2DHF form quantized states separated by a fraction of a meV. Edge states on steps between terraces appear along one of the two in-plane directions, suggesting electronic symmetry breaking at the surface. Our results propose a new route to realize quantum-well states in strongly correlated quantum materials and to explore how these connect to the electronic environment [1].

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Diversity of radial spin textures in chiral materials

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We introduce a classification of the radial spin textures in momentum space that emerge at high-symmetry points in crystals characterized by non-polar chiral point groups (D_2 , D_3 , D_4 , D_6 , T , O). These spin textures are an important ingredient to explain the current induced magnetization parallel to direction of the electric field, an effect that might find application in spintronics devices. Based on the symmetry constraints imposed by these point groups in a vector field, we study the general expression for the radial spin textures up to third order in momentum. Furthermore, we determine the high-symmetry points of the 45 non-polar chiral space groups supporting a radial spin texture. These two principles are used to screen materials databases for examples of systems that go beyond the basic hedgehog radial spin texture. As a result, we found that complex radial spin textures given by quadratic and cubic momentum terms are common in the band structure of any material with high-symmetry points having a non-polar chiral point group. More generally, the symmetry analysis proposed in this work is also valid for studying other vector properties in momentum space.

Extending the spin excitation lifetime of a magnetic molecule on a proximitized superconductor

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Magnetic molecules adsorbed on surfaces serve as a platform to individually address and manipulate spins. In order to be able to use these spins in quantum information processing and data storage, long spin-relaxation times is a prerequisite. Normally, coupling of the spin with the conduction electrons of metallic substrates quenches the excited state lifetime and leads to short relaxation times T_1 . However, the presence of superconducting pairing effects in the metal substrate can protect the excited spin from relaxation [1]. Upon adsorption on a superconducting surface and depending on the coupling of the unpaired spins with the substrate, several in-gap [2] and out-gap [3] states may arise, which can be studied with scanning tunneling microscopy and spectroscopy. In this study, we use a substrate of a few monolayers of gold epitaxially grown on top of an oxygen reconstructed 1×5 -V(100) surface to decouple the molecular spin of an iron-porphyrin-chloride from itinerant electrons. The gold film exhibits a proximitized superconducting gap with in-gap de Gennes-Saint James resonances, which protects molecular spin excited states and results into a lifetime of $\tau \approx 80$ ns. The spin lifetime decreases with increasing film thickness due to the gradual gap-closing by the in-gap states. Our results elucidate the use of proximitized gold electrodes for addressing quantum spins on surfaces, envisioning new routes for tuning the value of their spin lifetime.

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Figures

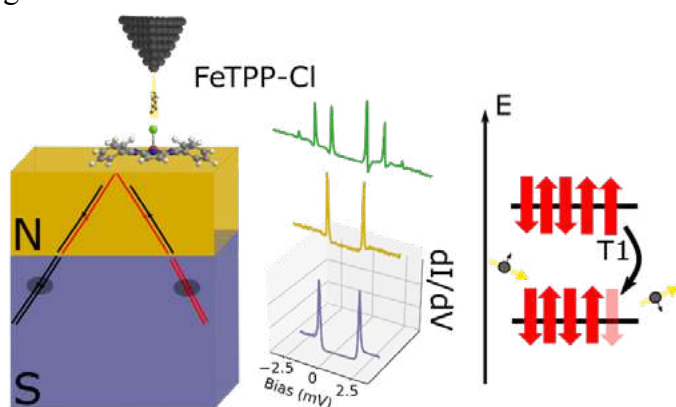


Figure 1: Left: Artistic description of the molecule/normal metal/superconductor system, Center: Corresponding spectroscopic signatures, Right: Illustration of a spin-flip excitation on the magnetic center induced by tunneling electrons

Real-Time Second Principles TD-DFT calculations of Optical Properties: Can large-scale methods be used to simulate Excitons?

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Research on solid-state spectroscopy is essential in the development of novel technological applications based on energy and charge transport. The phenomena observed in spectroscopy cover many topics in condensed matter as it is affected by the presence of impurities, distortion of the lattice (phonons) or electron scattering, and the results can be strongly dependent on the boundary conditions like strain or temperature. Analyzing the information obtained from experimental spectra can be difficult and supporting from *ab initio* calculations can be quite useful to interpret and understand the observations. However, this task is also a challenge as these simulations would require in many cases, large supercells, detailed sampling of atomic movement/impurity localization or require the use of advanced computational techniques to account for electron-electron and electron-hole correlations.

Therefore, it would be desirable to go beyond the capabilities of standard first principles methods to carry out predictive large-scale simulations. This fact motivates the development of a new family of methods, known as Second Principles (SP) [1], based on Density Functional Theory (DFT) and implemented in the code SCALE-UP. They allow large-scale material-simulations, including both atomic and electronic degrees of freedom, at a very modest computational cost. The method is based on the construction of models written in localized Wannier functions [2] and includes the capacity to describe the changes in the electronic state induced by the application of electric fields, variations in the geometry (including electron-phonon coupling) and the electron density itself (electron-electron scattering).

In this work, we show the results obtained by combining (i) the newly developed code to generate SP models, named MODELMAKER, and (ii) our implementation of real-time time-dependent DFT. Using our model generator, and based on hybrid DFT simulations, we are able to create models that take into account strong electron-electron interactions. Combined with our efficient algorithm to evolve the density matrix in real time (RT), we discuss the influence of these interactions after the system has been perturbed by a short electric pulse. Initial results show that electron-hole interactions have a strong influence on the resulting spectrum, and can be seen using our novel computational technique, unlike what happens in standard linear response TD-DFT calculations. This fact, indicates that RT-TD SP simulations could be a new powerful tool to study excitons at a computational cost much smaller than the one of the current methods like the Bethe-Salpeter equation.

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Synchrotron X-ray Coherence to Probe the Complexity of realistic interfaces at the Nanoscale

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The advent of the world's first coherent hard X-ray sources in France (ESRF) and the USA (APS) represents an unprecedented opportunity to conduct operando (i.e., in situ and time-dependent) studies on the structure and behavior of surfaces, interfaces, and single crystalline grains in reactive environments. In this talk, I will give an overview of the new approaches utilizing x-ray coherent scattering to observe the structure of crystalline matter in three dimensions and with special sensitivity to nanoscopic defects, lattice distortions, irregular morphologies and their evolution under experimental conditions mimicking natural environments. As an example, I will describe our recent studies about growth and dissolution at mineral-water interfaces with coherent x-rays. In the first study coherent X-ray reflectivity was used to reveal the morphology and the active sites for growth and dissolution of a an otavite (CdCO_3) thin film grown on a dolomite substrate [1]. The second study shows a novel approach to extract structural information from a coherent diffraction pattern based on the re-interpretation of the Patterson Function as an auto-hologram and a mathematical graph [2]. These two studies form the initial basis of a research program aiming to develop advanced coherent x-ray imaging methodologies to characterize the dynamic and chemical behavior of crystalline grains at the nanoscale and under realistic environments (e.g. mineral matrices, multilayered compounds, liquid solutions, etc.).

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Quantifying the magnetic anisotropy of 50 nm-magnetic nanoparticles embedded in biological entities

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Over the last years, the interest in nanomagnets have blown up aiming to overcome the fundamental need to develop novel nanotechnology-based pathways to achieve relevant performance in medicine. On the top of their reduced size, (comparable to those of proteins, nucleic acids, or viruses) that allows promising interaction with biological systems, the magnetic nature of the nanomagnets grants their manipulation by external magnetic fields. All of it makes magnetic nanostructures excellent candidates to be used as diagnostic agents, to locally heat and destroy cancer cells in hyperthermia cancer treatment or for targeted magnetic cell delivery in regenerative medicine [1]. All these applications rely on the underlying physical properties of the nanomagnets within the target biological entity. In particular, the role of the magnetic anisotropy arises an overriding question [2]. Despite its importance, the quantification of the magnetic anisotropy of individual magnetic nanostructures is a challenging task. Commonly used macroscopic magnetic characterization techniques average over hundreds or thousands of dissimilar nanomagnets, impeding to obtain reliable information about magnetic anisotropy of individual nanostructures. Regardless of the existence of magnetic sensitive microscopic methods, they are either limited in spatial resolution or in magnetic field strength or more relevant, they do not allow to measure magnetic signals of nanomagnets embedded in biological systems.

Here we present a hybrid experimental/theoretical method capable of working out the magnetic anisotropy constant and the magnetic easy axis direction of individual magnetic nanostructures down to 50 nm embedded in biological entities [3]. The method combines experimental data acquisition by means of scanning transmission x-ray microscopy using an axi-asymmetric magnetic field with theoretical simulations based on the Stoner-Wohlfarth model. The validity of the method has been tested over a model system consisting of single-domain intracellular magnetite nanoparticles biosynthesized by magnetotactic bacterium *Magnetovibrio blakemorei* MV-1. Magnetotactic bacterium MV-1 synthesize internally high-quality truncated hexa-octahedral magnetite (Fe₃O₄) nanoparticles with dimensions 35x35x65 nm arranged in chains. The elongated morphology of such particles along the chain direction (<111> direction), yields a strong effective uniaxial magnetic anisotropy along that direction [4]. As a consequence, the nanoparticles biosynthesized by *M. blakemorei* are uniaxial single magnetic domains whose magnetization process can be described by a modified Stoner-Wohlfarth model.

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Nanogenerators and self-powered sensors enabled by plasma and vacuum processing of multifunctional thin films and 3D nanoarchitectures

Ana Borrás

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Single- and multi-source environmental energy harvesters and nanogenerators will promptly pave the way for the realization of Industry 4.0 and Smart Cities. However, advances are yet required in the design of functional nanomaterials, and their synthesis and processing procedures. In this presentation, we will demonstrate the application of vacuum and plasma-assisted deposition techniques to process surfaces and thin films and to develop complex nanowires (NWs) and nanotubes (NTs) with a core@multishell morphology where each shell adds functionality or multifunctionality to the system. The steps required for the implementation of these nanomaterials as supported or in-device applications will be presented together with our latest accomplishments in the field of solar cells,[1-4] piezoelectric and triboelectric nanogenerators[5,6] and self-powered sensors.

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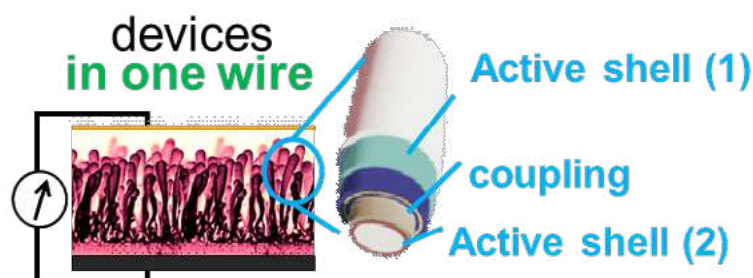


Figure 1: Schematic representation of a high-density array of multifunctional nanowires for multi-source energy harvesting.

STM Study and Electronic Transport Signature of Dithiahelicenes at Ambient Conditions

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Using a Scanning Tunneling Microscope (STM), we address the chiral molecules dithia[*n*]helicenes ([*n*]DTH, being *n* = 7, 9 and 11 the number of rings) in benzene solution [1, 2]. For each [*n*]DTH, two kinds were synthesized where the location of both sulfur atoms changes. This fact leads to different anchoring preferences.

For this work, Au(111) substrates were selected for studying the self-assembly of helicenes over the surface. First result shows differences during the deposition due to the interaction of the sulfur atom as a link group with the gold atoms. Moreover, we could image isolated molecules along their different binding configurations, measure the molecular diameter and establish a chiral recognition method at room conditions.

By means of STM-based BJ, we performed electronic transport measurements which show the most repeated conductance values when stretching the junction up to the formation of a molecular bridge.

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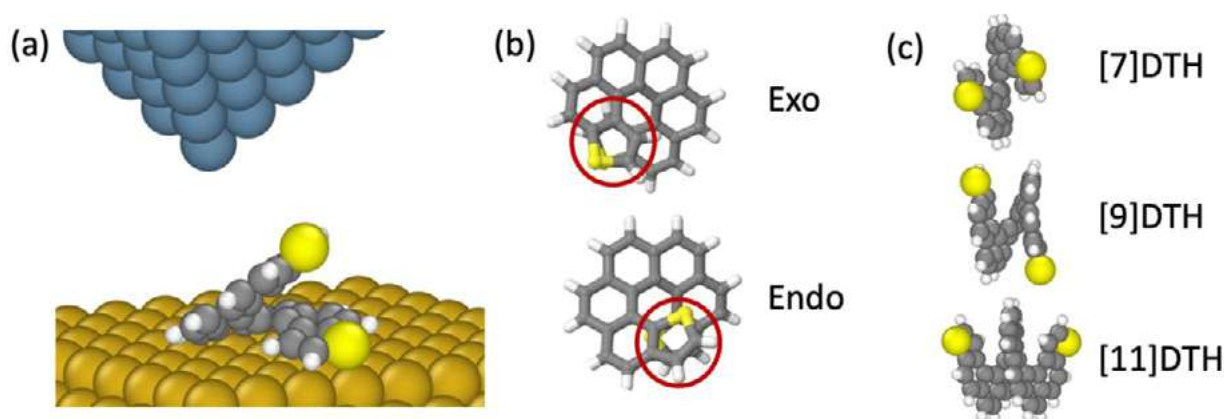
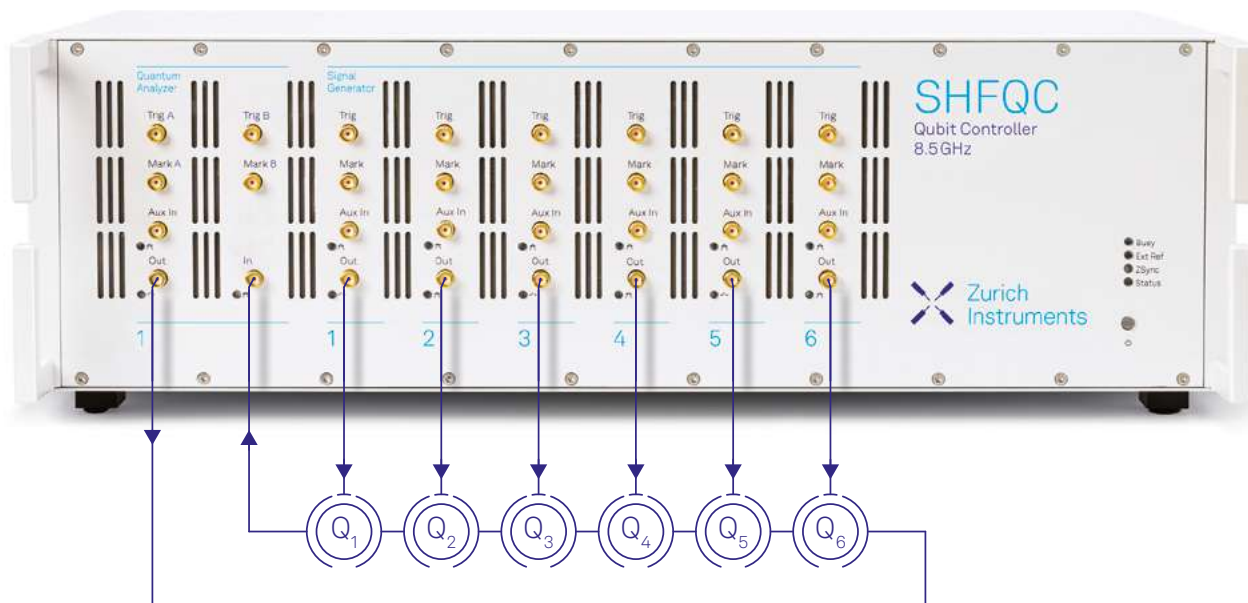


Figure 1: (a) Schematic illustration of an STM set up where a helicene is flat over a Au(111) substrate and the tunneling current is measured via a PtIr tip. For measuring via STM-based BJ, the tip is changed to a gold wire. Molecules are represented with grey, white and yellow spheres as C, H and S atoms respectively. The location of the sulfur atom is highlighted using a red circle for the exo and endo compounds in panel (b). Panel (c) shows a side view of one molecule as a function of *n*, being *n* = 7, 9 and 11 rings.

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Spatial control of the thermal conductivity in transition metal oxides

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Atomic point defects are one of the main sources of phonon scattering, and hence of the limiting factors of thermal conductivity in non-metallic crystals [1,2]. In the case of transition-metal oxides, an unavoidable number of ionized oxygen vacancies are formed during synthesis and remain randomly distributed along the crystal.

In some oxygen-deficient perovskites, previous experiments demonstrated that the electric field produced by a voltage-biased atomic force microscopy tip can induce a transformation between the perovskite and a brownmillerite phase at room temperature, with sub-micrometer spatial resolution.[3]

Here we show that such transformation can be exploited to produce different thermal conductivity states. In particular, we show that the thermal conductivity of several oxides can be modified $\approx 30\%$ at room temperature, with micron-size spatial resolution. This shows that ionic-based thermal devices can be fabricated by electric-field patterning.

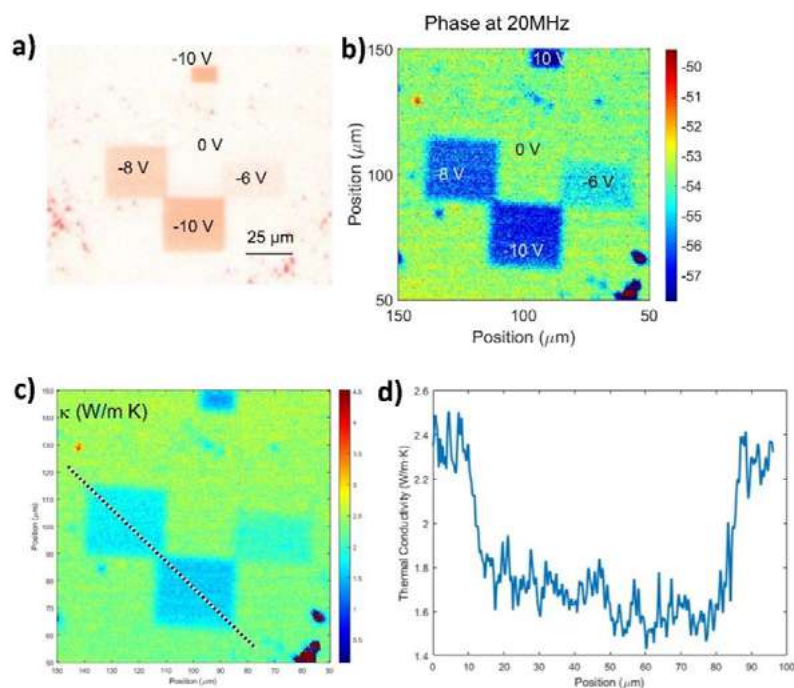


Figure 1: a) Atomic Force Microscopy image of a thin film of SrFeO_{3-x} deposited on STO. The dark squares have been scanned with a voltage-biased AFM tip, dragging oxygen vacancies and inducing the local transformation to the brownmillerite SrFeO_{2.5} phase. b) Frequency Domain Thermoreflectance Phase at 20 MHz obtained in the same region as a). In c) we show the thermal conductivity map obtained from the fitting of the reflectivity map. d) thermal conductivity along the dotted line shown in c).

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**POSTER
SESSIONS
PRESENTERS**

Poster Session A. Wednesday February 1st (morning and afternoon)

A.1 Yong Xie:

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

A.2 Abel Martinez-Suarez:

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

A.3 Jorge Cervantes Villanueva:

Strong exciton-phonon coupling in semiconducting monolayer 2H-MoTe₂

A.4 Maria José Calderón:

Electronic correlations in the normal state of twisted bilayer graphene

A.5 Sergio Pezzini:

Twisted devices from CVD graphene

A.6 Eduardo B. Molinero:

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

A.7 Gabriel Caballero Catalan:

Memristive behaviour in exfoliated and nanostructured three-terminal MoS₂ devices

A.8 Julia García Pérez:

Performing an array of MoS₂ micro-drum resonators

A.9 Marcos Gadea García:

Highly tunable opto-electrical response in FePS₃-MoS₂ van der Waals p-n heterojunctions

A.10 Carlos Sánchez Sánchez:

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

A.11 Eudomar Henriquez Guerra:

Photo-thermoelectric effect in MnBi₂Te₄ devices revealed by scanning photocurrent microscopy

A.12 Enrique Terán García:

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

A.13 Juan Salvador Sánchez:

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

A.14 Manuel Suárez Rodríguez:

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A.15 Gonzalo Álvarez Pérez:

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

A.16 Cristina N. Hernández Fuentevilla:

Spin filtering induced by a magnetic insulator stripe on graphene

A.17 Inés Sánchez de Movellán Sáiz:

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A.18 Pablo Moles Matías:

Electronic transport through twisted bilayer graphene flakes with defects

A.19 María Rodríguez Losada:

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

A.20 Jan Phillips:

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

A.21 Karolina Z. Milowska:

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A.22 Marcel S. Claro:

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A.23 Joan Ripoll Sau:

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A.24 Vittorio Bellani:

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A.25 M. Dolores Merchán:

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A.26 José López Molina:

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A.27 Gulsum Ersu:

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

A.28 Thomas Pucher:

High-mobility MoS₂ phototransistor using biodegradable albumen dielectrics

A.29 Reyes Calvo:

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A.30 José Alejandro Ruiz Torres:

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A.31 Adrián Arenas Gulló:

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A.32 Esther Barrena:

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A.33 Jose M. Pereira:

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A.34 Ignacio Gimeno:

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A.35 Jaime Bueno Benito:

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A.36 Ana Isabel Fernández-Tresguerres:

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A.37 Carlos Sabater:

Molecular electronics: insight from simulations and calculations

A.38 Manuel Martín Bravo:

An apophatic description of spherical shells

A.39 Maximilian Bailey:

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A.40 César Pascual García:

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A.41 Ramón Planet:

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A.42 Alejandro Rivelles:

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A.43 Oscar Iglesias:

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A.44 Jinan H. Al Shuhaib:

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A.45 Maha Labani:

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Ga₂O₃:Cr nanowire-based optical microcavities for thermometry

A.48 José Balduque Picazo:

Resonant tunneling energy harvesters: improving performance via quantum interference

A.49 Ramón Bernardo Gavito:

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

A.50 Emilio Artacho:

Floquet theory of electronic stopping of nuclear projectiles in solids

A.51 David Hernández Pinilla:

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

A.52 Jorge Quereda Bernabeu:

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A.53 Rania Daoudi:

Photoluminescence properties of carbon nanodots with high nitrogen level

A.54 Óscar Pozo Ocaña:

Multipole description of optical spatial dispersion in crystals

A.55 Julia García Prieto:

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

A.56 Ignacio López Quintás:

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

A.57 Yuriko Baba:

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

A.58 José Álvarez Cuervo: Twistoptics:

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

A.59 Sebastián Roca Jerat:

Suppression of superradiance by magnetic correlations

A.60 Javier Fernández Martínez:

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A.61 Miguel Ángel Sánchez Martínez:

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

A.62 Alberto Rodríguez:

Quantum chaos in the Bose-Hubbard model

A.63 Andrei Bylinkin:

Hyperbolic light interacting with molecules

A.64 Rodrigo de Paula Almeida Lima:

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A.65 Luis Brey:

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A.66 Pepa Martínez-Pérez:

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A.67 Marta García Olmos:

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A.68 Vito Clericò:

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A.69 M. Pilar López Sancho:

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A.70 Jose Antonio Moreno:

Scanning Tunneling Spectroscopy in topological Dirac semimetal ZrTe₅

A.71 Raquel Sánchez Barquilla:

Electronic band structure and atomic level Landau quantization in the type-II Weyl semimetal WTe₂ visualized by Scanning Tunneling Microscopy

A.72 Hayden Salway:

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

A.73 Juan José Esteve-Paredes:

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

A.74 Andrea Peralta Somoza:

Large topological Hall effect and spin textures in La_{0.7}Sr_{0.3}MnO₃ / SrIrO₃ bilayers

A.75 Javier Martín Sánchez:

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

A.76 Hernán Santos:

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

A.77 Jorge Alejandro Budagosky Marcilla:

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A.78 Josu Diego López:

Mechanical and acoustic properties of graphene explained thanks to anharmonic effects

A.79 Aitana Tarazaga Martín-Luengo:

Multiple and spectrally robust photonic magic angles inreconfigurable α -MoO₃ trilayers

A.80 Elena Pinilla:

Accurate transfer of individual nanoparticles onto single photonic nanostructures

A.81 Javier Rodríguez:

Interaction-driven Circular Dichroism through absorption modes in Triskelia Nanostructures

A.82 Marta Fernández Lomana:

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A.83 Carla Boix-Constant:

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A.84 Alessandro James Mirabelli

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B.2 Meritxell Toda:

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B.3 Amina Hadjoudja:

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B.4 Diego Caso:

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B.5 Zahia Ferhat:

Exchange bias alteration mediated by layers with perpendicular magnetic anisotropy

B.6 Amina Mazouz:

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B.7 Pablo Camarero Linares:

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B.8 Víctor Zamora:

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B.9 Irián Sánchez Ramírez:

(TaSe₄)₃I: Reconciling transport, optics and ARPES

B.10 Rafael Delgado García:

Magnetization Reversal Processes of Highly Anisotropic Corrugated Thin Films

B.11 Isabel Barbero Velasco:

NdNiO₃-BaTiO₃ Ferroelectric Tunnel Junctions

B.12 Andrea Aguirre Baños:

Tunable ferromagnetic order in 2D layered transition metal dichlorides

B.13 Fernando Gallego Toledo:

Study of Spin-to-charge conversion effect in ferromagnet/2DEG based nanodevices: The reading section of the MESO device

B.14 Ana García-Page:

Dragging of Berry curvature in ferromagnetic Weyl semimetals NiMnSb and PtMnSb

B.15 Lucía Martín Pérez:

Direct magnetic evidence, functionalization and low-temperature magneto- electron transport in liquid-phase exfoliated FePS₃

B.16 Fernando Luis:

Size-dependent dipolar ferromagnetism in micro- and nano-molecular crystals

B.17 Nayara Carral Sainz:

Automatic procedure to obtain tight-binding parameters for second- principles simulations. The case of SrTiO₃

B.18 Julia Herrero-Albillos:

Optimizing the performance of IrO₂ thin films by doping with Co

B.19 Marcel S. Claro:

Thermal transport on few-layers Fe₃GeTe₂

B.20 Lucas Pérez:

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B.21 Isabel Tenreiro:

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B.22 Montserrat Xochitl Aguilar Pujol:

Magnon currents excited by the spin Seebeck effect in ferromagnetic EuS thin films

B.23 Isabel Cristina Arango Gutierrez:

Spin-to-charge conversion in Bi₂Se_{1-x} from all-electrical nanostructured devices

B.24 Jone Mencos Frechilla:

Looking for the spin swapping effect

B.25 Yaiza Asensio García:

Modulating the magnetic properties of layered hybrid organic-inorganic metal-halide perovskites by chemical design

B.26 Daniel Tezze:

Tuning the magnetism of NiPS₃ and MnPS₃ through organic ion intercalation

B.27 Marcos Rubín Osanz:

Decoherence-free molecular spin qubits with chemically designed frequencies

B.28 Miguel Moreno Ugeda:

Superconducting dome by tuning through a Van Hove singularity in a two-dimensional metal

B.29 Ignasi Fina Martínez:

Stress effects on ferroelectric doped epitaxial HfO₂ oxide films and its impact on functional properties

B.30 Gabriel Rodríguez Rodríguez:

Low temperature MFM characterization of adjustable 3D ferrimagnetic NdCo/GdCo/NdCo trilayers

B.31 Adriana I. Figueroa:

Probing strain-induced ferromagnetism in epitaxial SrMnO₃ films

B.32 Ana Parente:

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B.33 Yelko del Castillo Hernández:

Certifying entanglement of spins on surfaces using ESR-STM

B.34 Javier García Alonso:

In-situ characterization of NMC particles with applications in Li-ion batteries

B.35 José Joaquín Pérez Grau:

Layer-dependent evolution of the optical properties in 2D CrI₃ mapped by hyperspectral imaging

B.36 Jesús Ortega Fibla:

Dislocations in GaN on sapphire for power applications: an ultraviolet light-assisted Kelvin probe force microscopy study

B.37 Laura Fernández García:

Magnetic Domain Wall Ferromagnetic Resonance Confirmed by Magnetotransport Measurements and Kerr Microscopy

B.38 Patricia Ferrer Alcaraz:

A Versatile 3D Printable Scanning Tunneling Microscope

B.39 Emanuel Alberto Martínez:

Observation of an anisotropic two-dimensional electron gas at the (110) surface of KTaO₃

B.40 Alejandra Guedeja-Marrón:

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B.41 Fran Romero-Lara:

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B.42 Juan de la Figuera:

Angle Resolved Reflection Electron Spectroscopy in a Low-Energy Electron Microscope: the path to map the unoccupied states in the Nanoworld

B.43 Antonio David Subires Santana:

Electronic band structure of the Co pnictide A(CoX)₂ (A=Ca, Eu and X=As, P) probed by ARPES

B.44 Flavio Bruno:

A Laser-ARPES View of the 2D Electron Systems at LaAlO₃/SrTiO₃ and Al/SrTiO₃ Interfaces

B.45 Mariela Menghini:

Magneto-transport properties and anomalous Hall effect in ferromagnet/nanostructured superconductor hybrid systems

B.46 Rodrigo Guedas García:

Exploring current limits without damaging nanostrips

B.47 Ignacio Casal:

Characterization of superconductivity in Full-Shell Al/InAs Nanowires

B.48 Stefano Trivini:

Competition of Superconducting and Coulomb Correlations in Pb islands on graphene

B.49 Beatriz Rodríguez Fernández:

Rapid synthesis by Joule heating of low-dimensional transition metal oxide materials

B.50 Jon Ortuzar Andres:

Magnetic molecule as a parity sensor in entangled spin and YSR excitation on a superconductor

B.51 Guillermo López-Polin:

Energy harvesting from Anomalous Nernst effect on Co/Pt multilayers

B.52 Ignacio Figueruelo Campanero:

Fabrication and characterization of exfoliated high-temperature superconductor Bi₂Sr₂CaCu₂O₈ flakes for van der Waals heterostructures

B.53 Carlos Untiedt:

Study of the Electrical Capacitance From Classical to the Quantum Regimen

B.54 Cristina García Pérez:

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B.55 Alessio Vegliante:

Engineering π -Magnetism in Carbon-Based Nanostructures

B.56 David Rodríguez:

Electron paramagnetic resonance spectrometer based on lumped element superconducting resonators

B.57 Marina Calero de Ory:

Bridging spin Qbits to superconducting circuits through carbon nanotubes to superconducting circuits through carbon nanotubes

B.58 Alicia Gómez:

High cooperativity coupling to nuclear spins on a circuit quantum electrodynamics architecture

B.59 Ana Pérez Rodríguez:

Effect of gallium doping on structural and transport properties of topological insulators Bi₂Se₃ by MBE

B.60 Elena Díaz García:

Spin-dependent polaron transport in helical molecules

B.61 Víctor Rouco:

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B.62 Jorge Estrada Álvarez:

Electronic properties of topological rough nanowires for thermoelectrical performance

B.63 David García Pons:

Fabrication of a nanoSQUID for the study of quantum magnonics

B.64 Dunkan Martínez Camacho:

Traces of Majorana zero modes in spin-polarized persistent currents

B.65 Daniel Muñoz-Segovia:

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B.66 José María De Teresa:

Josephson junctions and nanoSQUIDs grown by Focused Ion Beam Induced Deposition (FIBID)

B.67 Manuel Pino García:

On the capacitive coupling of persistent current qubits

B.68 Jorge Pérez-Bailón:

Development of replicable SQUIDs from the control of the fabrication of Nb-based dayem bridge junctions

B.69 Santiago Blanco Canosa:

Suppression of the CDW and SC orders and emergence of short-range magnetic order in 6R-NbSeTe

B.70 Pablo Canca López:

Study of defects under irradiated Fe through ab-initio techniques: cementite – Fe bcc interfaces

B.71 Alex Francisco Estupiñán López:

Simulations of a micro positioner and PCB design for measurement of SQUIDs

B.72 Carlos Uriarte González:

The Interaction of a Levitating Sphere with Helium Superfluids

B.73 Ramon Aguado:

Quantum dot Josephson junction in a hybrid superconductor-semiconductor transmon device: a novel route for Andreev spin qubits

B.74 Pedro Alcázar Guerrero:

Spin Relaxation in corrugated Graphene

B.75 Pilar García Estevez:

The singular manifold method and soliton-like solutions for Nonlinear Schrödinger Equation

B.76 Luis Manuel Canonico Armas:

Hot electron dynamics in graphene – a linear-scaling atomistic approach

B.77 Linda A. Zotti:

Metal-Protein-Metal Junctions: Electron Transport and Mechanical Deformation

B.78 Enrique Burzurí:

Magnetically-diluted two-dimensional CoII RhIII bimetallic oxalates as quantum spin liquid candidates

B.79 Celia González Sánchez:

Towards hybrid van der Waals Josephson junctions based on NbSe₂

B.80 Enrique Guzmán:

Electronic transport experiments and topography images in Tellurium

B.81 Marta Fernández-Lomana Gómez-Guillamón:

Tunneling spectroscopy at very high magnetic fields in the iron based superconductor KFe₂As₂

B.82 Pablo García Talavera:

Superconductivity and band structure of AuSn₄

B.83 Miguel Águeda:

Tunneling spectroscopy through the magnetic phases of Ce(Ru_{0.92}Rh_{0.08})₂Si₂

B.84 Beilun Wu:

Magnetic field induced increased d-electron overlap in Au-Au junctions

B.85 Alejandro José Uría:

Topological phase diagram of amorphous 2d Bi_xSb_{1-x} alloys from its entanglement spectrum

B.86 Ángel Ibabe:

Joule heating effects in superconducting InAs nanowire islands

B.87 Verónica Salgueiriño:

Spin-phonon coupling in antiferromagnetic Cr₂O₃ Nanocrystals

B.88 Manuel Antonio García Blázquez:

A group-theoretic approach to chirality-induced spin selectivity in molecular junctions

B.89 Adam Roselló:

Nanopatterning of hBN/WSe₂/hBN heterostructures for photonic applications

B.90 El Hadj Abidi:

Plasmonic Rectification of terahertz radiation using encapsulated graphene field effect transistor

B.91 Miguel Anaya:

Directional Light Amplification in Perovskite LEDs by Hybrid Photonic-Plasmonic Modes

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**POSTER
SESSION
A
WEDNESDAY,
FEB 1**

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

Yong Xie^{1,2*}, Haitao Yang², Kexin He², Daniel Yélamos¹, Eduardo Robert Rafael Hernández¹, Andres Castellanos-Gomez¹

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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 (MoS₂) collected by optical microscopy (OM), the semantic segmentation convolutional neural network (CNN) is used to achieve accurate recognition and rapid identification of MoS₂ 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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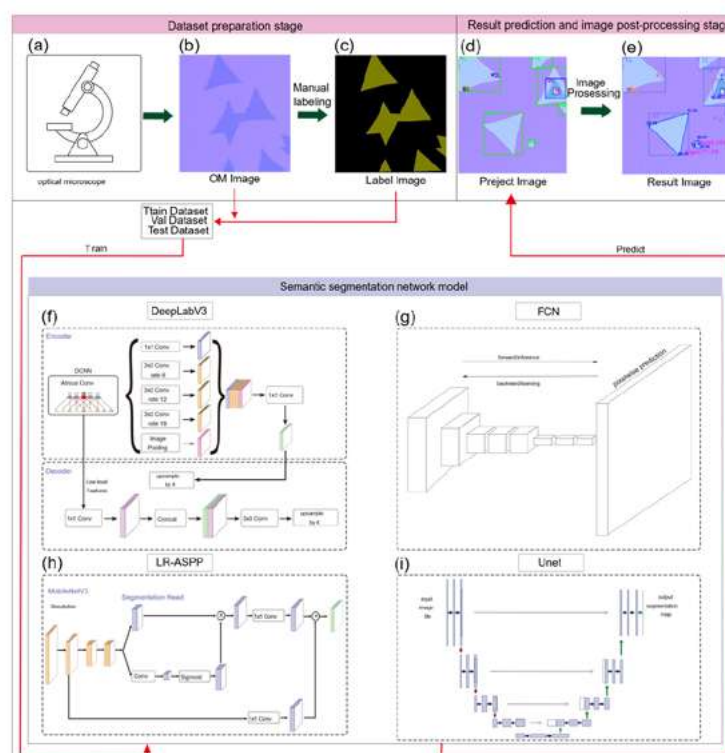


Figure 1: The process of identification of twisted bilayer TMDs.

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-Luengo¹, Stefan Partel⁴, Sandra Stroj⁴, Pablo Alonso-González^{1,2}, Javier Martín-Sánchez^{1,2}

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²*Nanomaterials and Nanotechnology Research Center (CINN-CSIC), El Entrego, Spain*

³*Donostia International Physics Center (DIPC), Donostia/San Sebastián, Spain*

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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 irradiated 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 $2H\text{-MoTe}_2$

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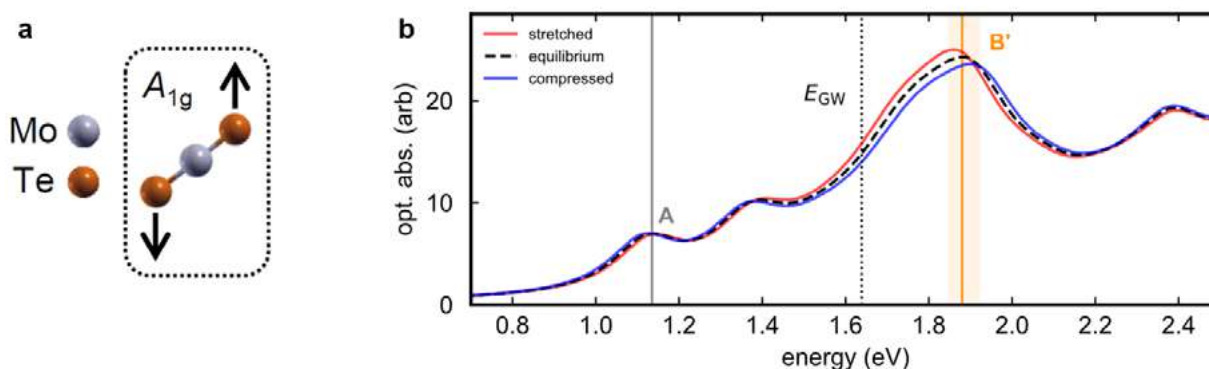
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The coupling of the electrons to lattice vibrations and their time-dependent control and detection provides unique insight into the non-equilibrium physics of semiconductors. $2H\text{-MoTe}_2$ is a transition metal dichalcogenide (TMD) that has not 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 $2H\text{-MoTe}_2$ 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

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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

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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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Figures

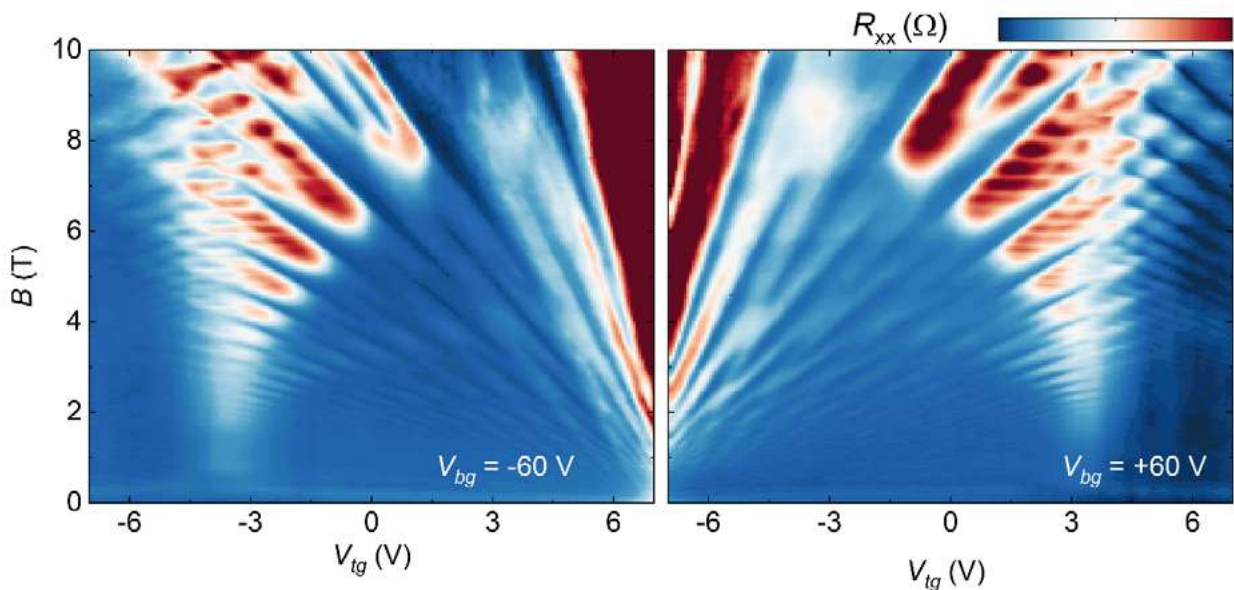


Figure 1: Longitudinal resistance of 2.4° -twisted bilayer graphene as a function of the top-gate voltage (at two different back-gate values), and the magnetic field. Oppositely-dispersing Landau fans coalesce at low-energy van Hove singularities (light red funneling regions). Density-independent Brown-Zak 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.

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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 graphene 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 appearance 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 survive 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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Figures

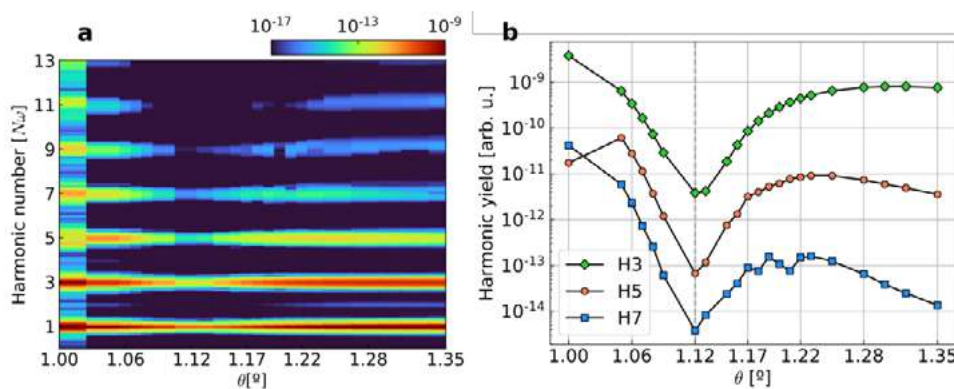


Figure 1: **a**, harmonic intensity in terms of the twist angles and the harmonic number. **b**, harmonic yield for the third, fifth and seventh harmonics in terms of the twist angles.

Recent Advancements in Lab-based 3D and 4D X-ray Microscopy of Materials at the Nanoscale

Carl Zeiss RMS, Oberkochen, Germany



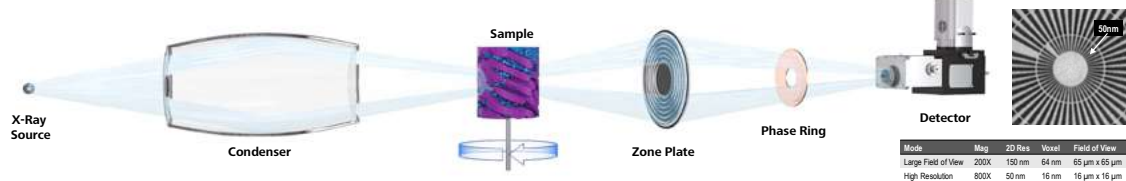
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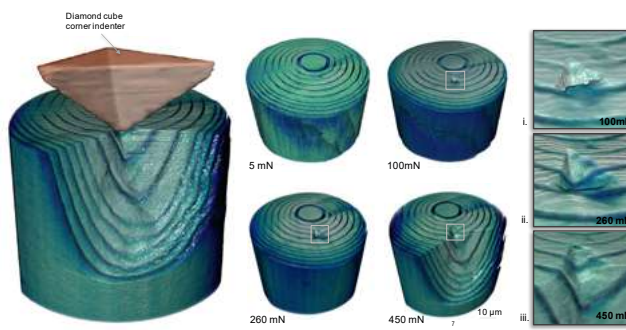
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Synchrotron quality optics. Laboratory accessibility.

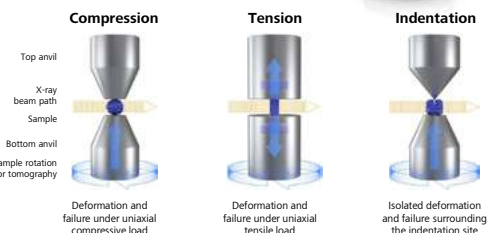


In Situ Nano-Indentation of a Single Fiber

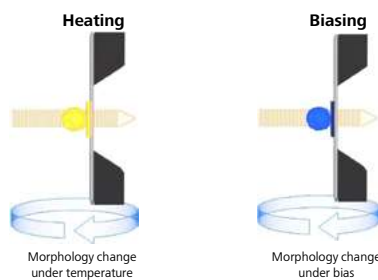


Silicon carbide fiber imaged while subjected to indentation load *in situ*

Xradia Ultra Load Stage

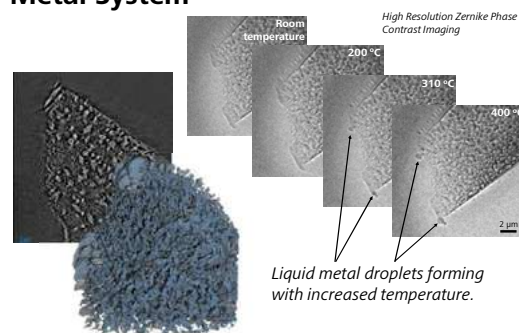


Norcada Heating Stage for Xradia Ultra



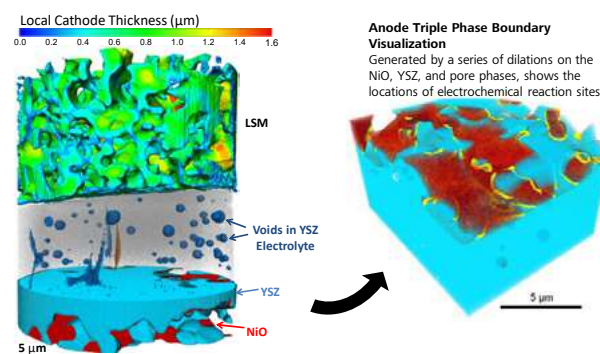
In situ sample heating from RT – 500 °C and sample biasing through MEMS chip technology.

Supported Catalytically Active Liquid Metal System

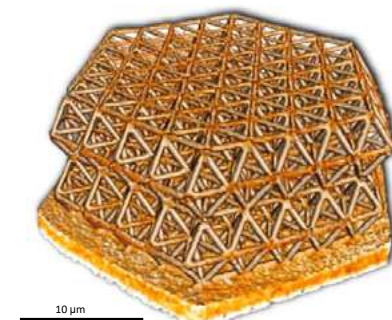


Liquid metal droplets forming with increased temperature.

Characterizing Solid Oxide Fuel Cell Microstructure



Polymer Nanolattice



3D printed nanolattice structure imaged in Zernike Phase Contrast before in situ compression experiments. Sample courtesy of Ruth Sweiger, KIT

Memristive behaviour in exfoliated and nanostructured three-terminal MoS₂ devices (Times New Roman 15)

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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 MoS₂ 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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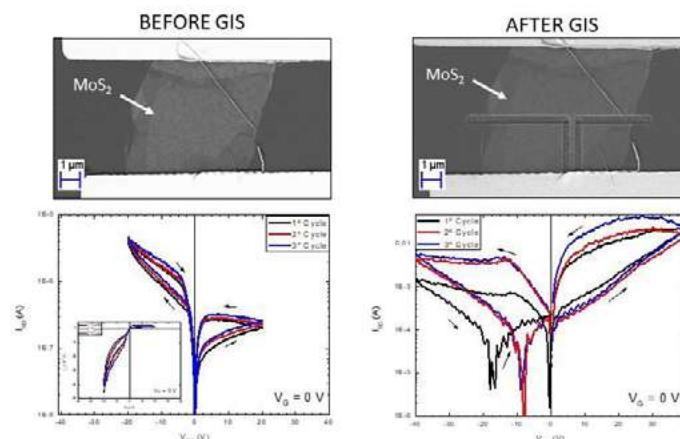


Figure 1: Characteristic curves before and after nanopatterning process.

Performing an array of MoS₂ micro-drum resonators

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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 MoS₂.

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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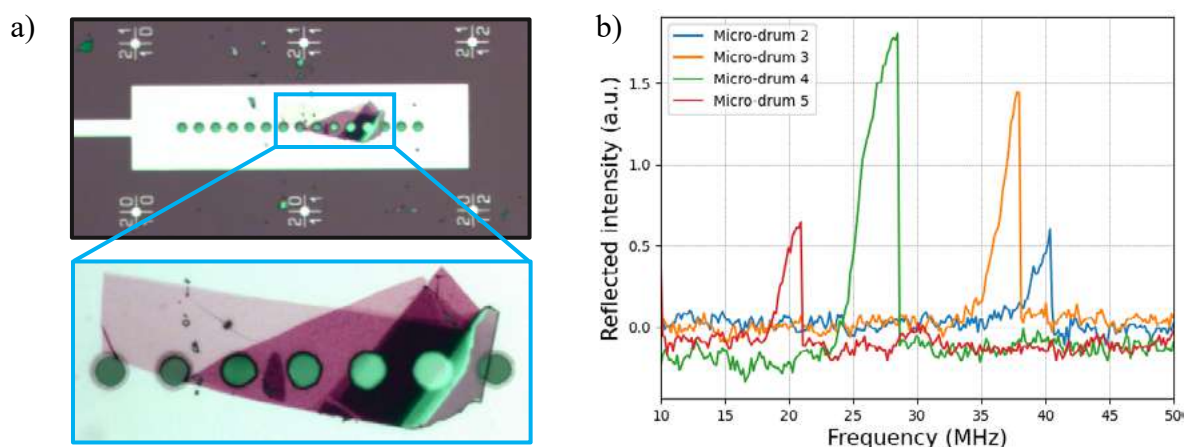


Figure 1: a) Micrograph of the system. MoS₂ flake with different number of layers onto five well-defined wells. b) Resonance frequency of four micro-drum.

Highly tunable opto-electrical response in FePS₃-MoS₂ van der Waals p-n heterojunctions

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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 MoS₂ and p-type, multilayer FePS₃, 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 FePS₃/MoS₂ 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 MoS₂ 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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Figures

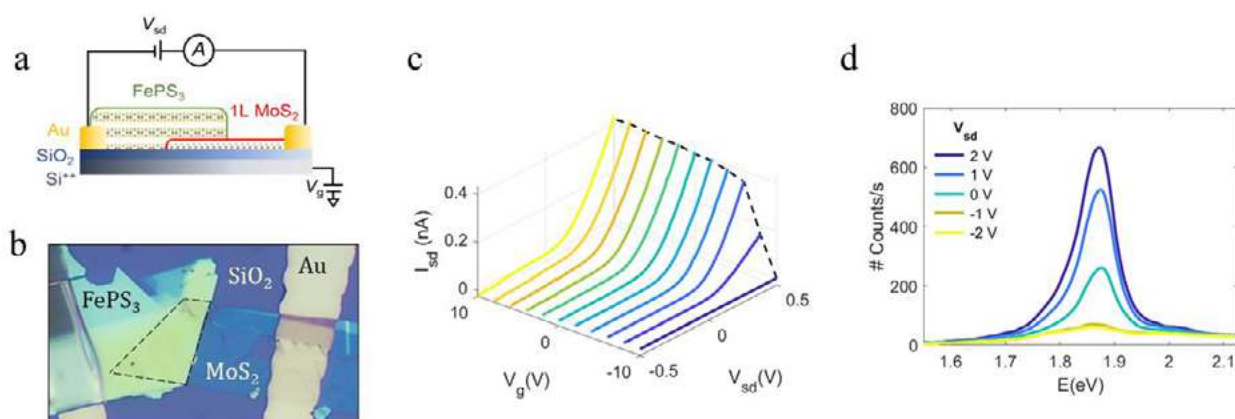


Figure 1: (a) Sketch for a device containing a multilayer FePS₃/ single-layer MoS₂ heterostructure. (b) Optical microscopy image of a heterostructure device (c) Source-drain current-voltage characteristics as a function of the applied back-gate voltage. (d) Photoluminescence emission of single-layer MoS₂ composing the FePS₃-MoS₂ heterojunction as a function of the applied bias voltage.

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

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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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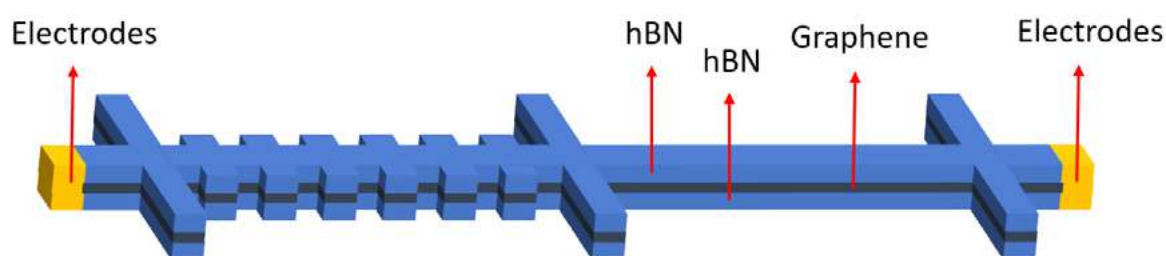


Figure 1: Image of the hBN-Graphene-hBN heterostructure device. The gate-defined channel contains two sections: a 2.5- μm -wide and 25- μm -long straight channel and a crenellated channel of the same dimensions with crenellations of 1 μm . In the crenellated channel, electrical resistance in the hydrodynamic 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

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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 $\sim 100\text{nm}$ 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 ($\lambda=532\text{nm}$) is placed on the $\text{MnBi}_2\text{Te}_4/\text{Au}$ 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

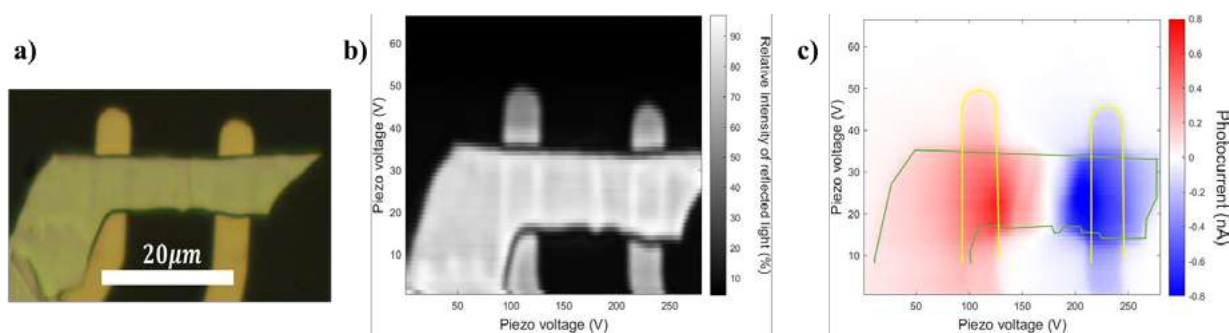


Figure 1: a) Optical microscopy image of a MnBi_2Te_4 device. b) Confocal microscopy map recorded simultaneously to c) Scanning photocurrent map for the device in a).

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

Enrique Terán García

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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

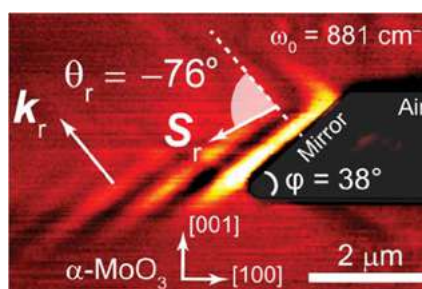


Figure 1: Visualization of negative reflection of nanoscale-confined polaritons in a natural medium.

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

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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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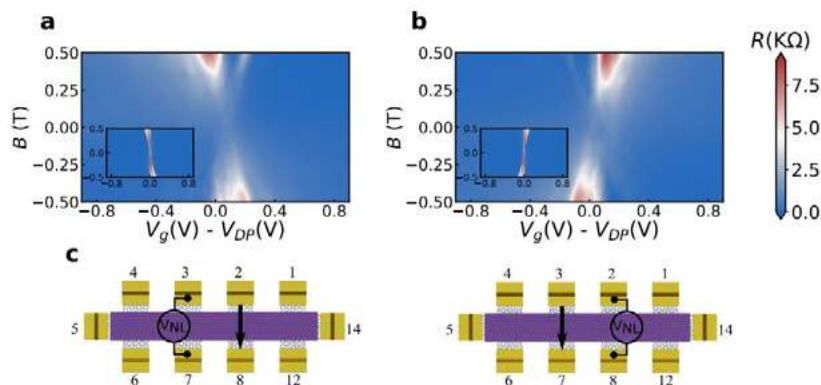


Figure 1: Panels **a** and **b** show the heat maps of the sample non-local resistance for two symmetrical configurations scanned in the space of backgate voltage, corrected by the position of the Dirac peak at $B = 0$ ($V_g - V_{DP}$), and magnetic field measured at 250 mK. Insets on each graph show 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

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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 constraints 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.

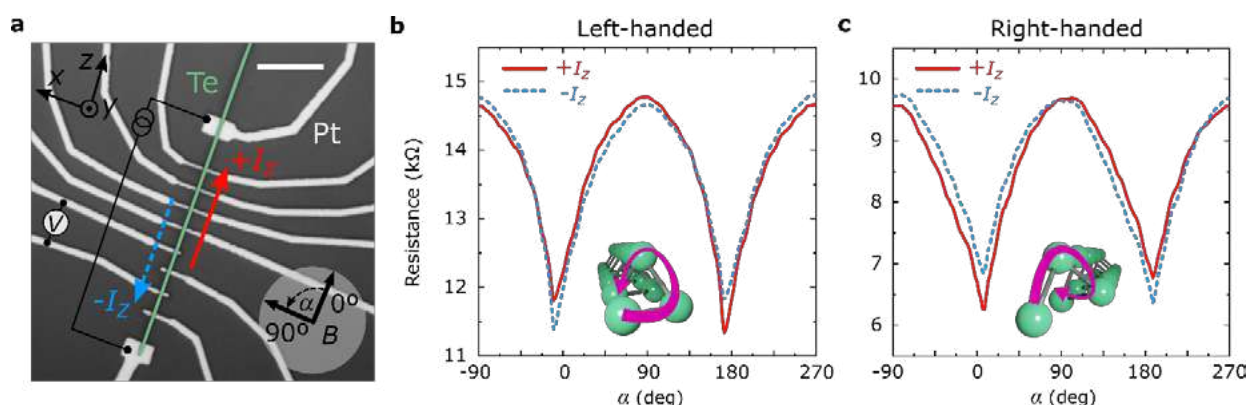


Figure 1: **a**, Te NW contacted with Pt contacts (the scale bar corresponds to 10 μm). **b,c**, Angular dependences of the magnetoresistance measured at 9 T and 10 K for two Te NWs with opposite handedness. Solid and dashed lines indicate the signal obtained from opposite current directions ($\pm I_z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

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

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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

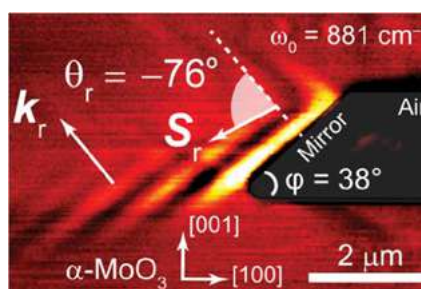


Figure 1: Visualization of negative reflection of nanoscale-confined polaritons in a natural medium.



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Spin filtering induced by a magnetic insulator stripe on graphene

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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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Figures

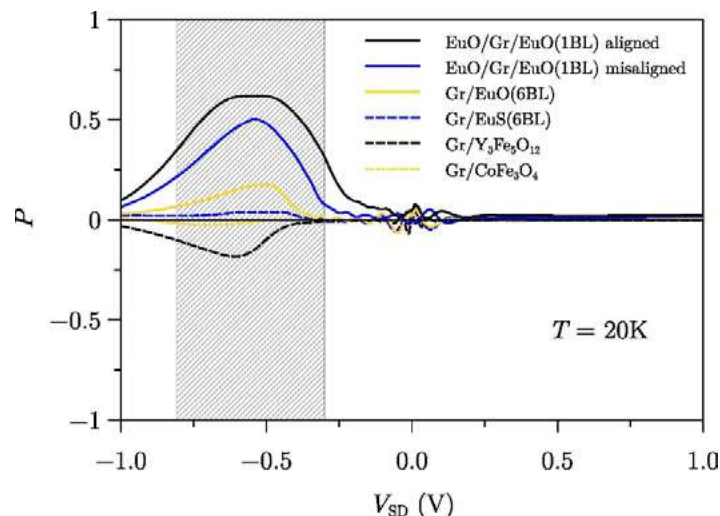


Figure 1: Current density polarization P as a function of the source-drain voltage V_{SD} for different FMI, when $U_0 = 500$ meV and $L = 50$ nm.

Structure and properties of layered materials: role of orthorhombic instability

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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 $(\text{C}_2\text{H}_5\text{NH}_3)_2\text{CdCl}_4:\text{Cu}^{2+}$ 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].

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Electronic transport through twisted bilayer graphene flakes with defects

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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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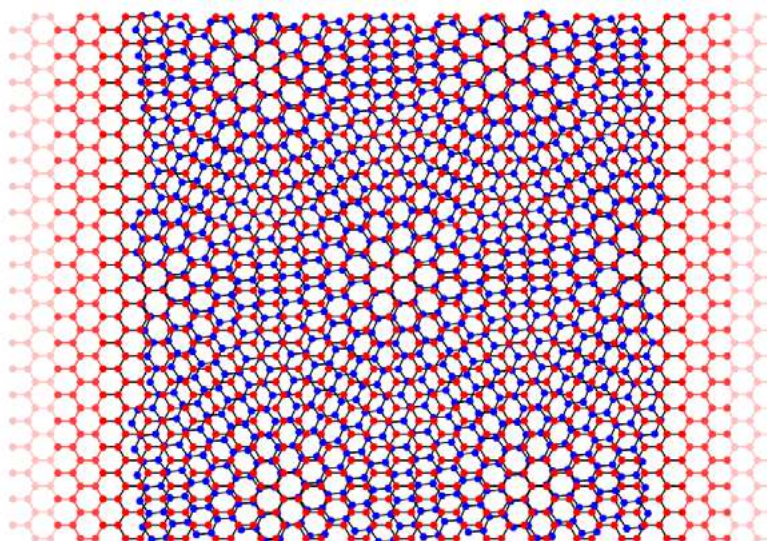


Figure 1: Twisted bilayer graphene flake contacted by two leads.

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

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In this work¹, 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.

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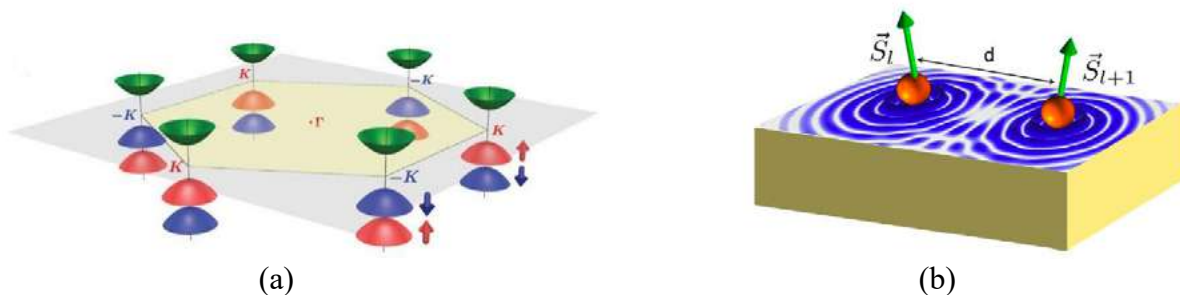


Figure 1: (a) Schematic drawing of the spin-valley coupled band structure (Picture taken from [5]). (b) Scheme of the mechanism of the indirect exchange interaction between two localized surface spins (Taken from [6])

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

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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.

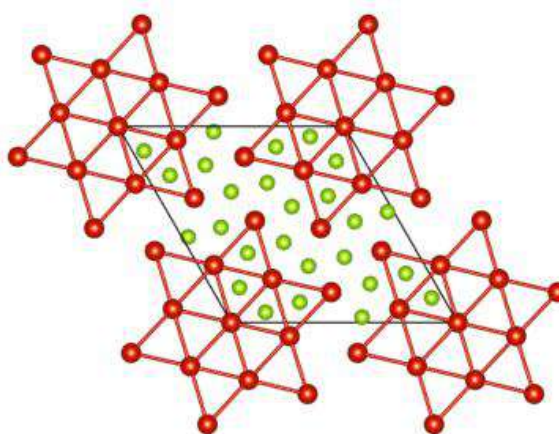


Figure 1: David star CDW phase for a transition metal dichalcogenide. The transition metal atoms are represented in red, while the chalcogene atoms are represented in green.

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

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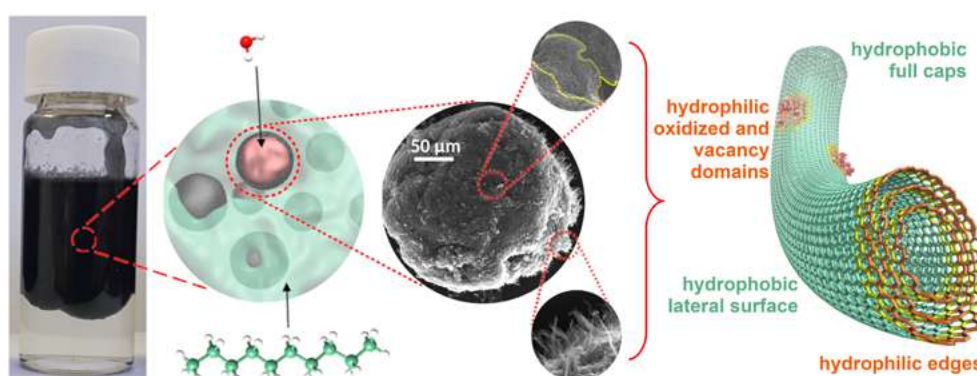
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Carbon nanotubes (CNT)s have already demonstrated scientific and technological breakthroughs including scalable coatings, composites, supercapacitors, tissue engineering, and biosensors. However, inconsistencies in understanding of water-solid interfaces 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 aquatotoxic 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

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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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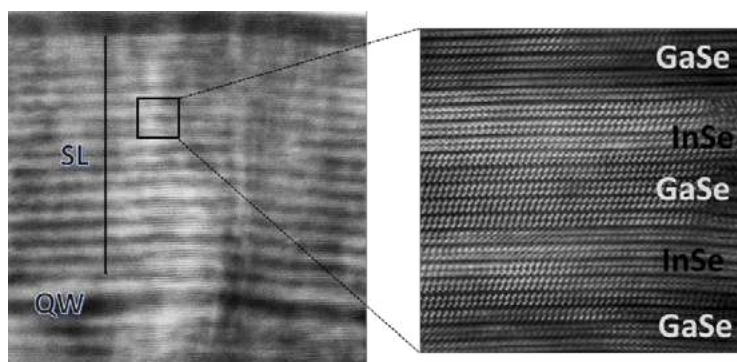


Figure 1: Cross-sectional view by Transmission Electron Microscopy (TEM) of 2.5nm GaSe/ 2.5nm InSe superlattice(in detail) embedding a quantum-well (on Sapphire substrate).

Phase engineering of two-dimensional Transition Metal Ditellurides

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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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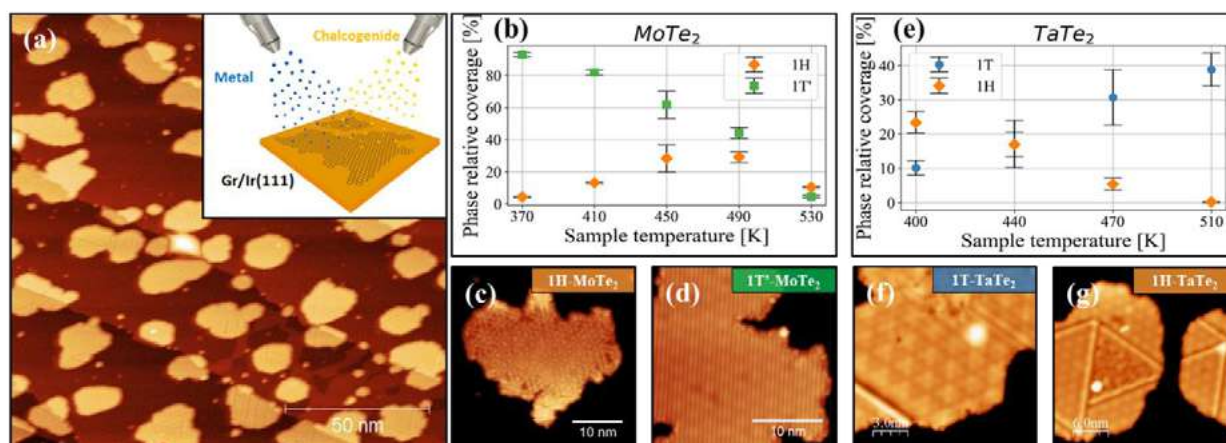


Figure 1: (a) Large STM image of TaTe_2 islands on gr/Ir(111) ($V = -1\text{V}$; $I = 0.1\text{nA}$). Inset: sketch of the growth procedure. (b) Relative coverage of 1T' vs. 1H- MoTe_2 phases for different growth temperatures. STM images of (c) 1H- MoTe_2 ($V = 0.5\text{V}$; $I = 0.1\text{nA}$) and (d)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

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

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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 $250.000 \text{ m}^2\text{V}^{-1}\text{s}^{-1}$, 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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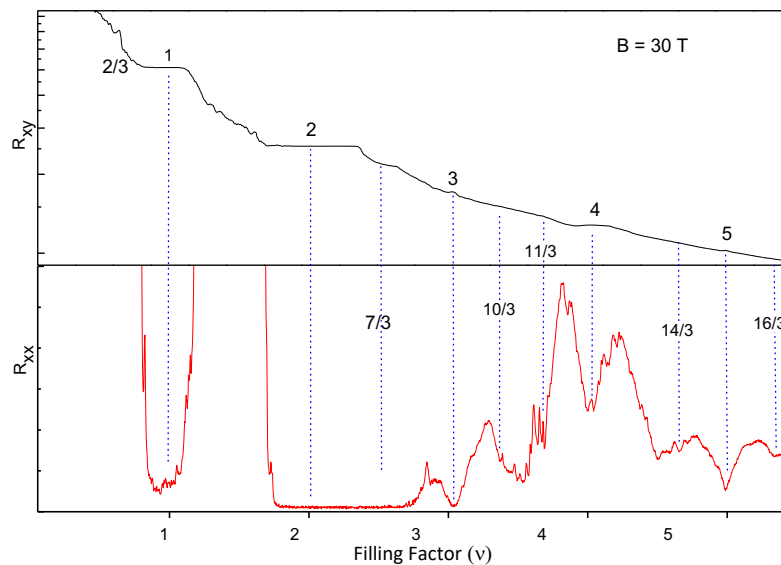


Figure 1: Integer quantum Hall states and composite Fermions in the Moiré landscape.

Synthesis and characterization of hybrids materials of transition metal oxides and graphene oxide. Evaluation of their properties as CO₂ adsorbents and as supercapacitor electrodes

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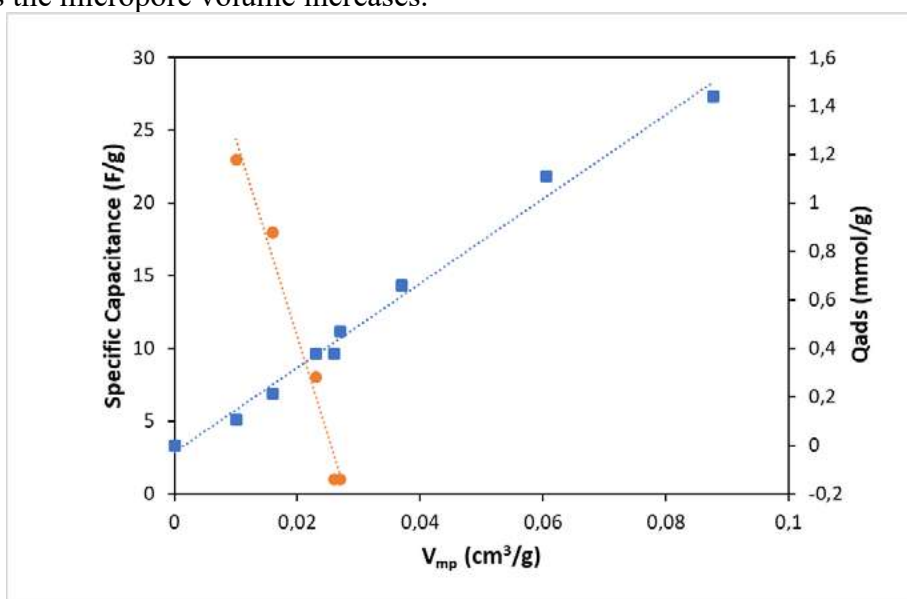
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Graphene-based hybrid materials have been prepared by incorporating inorganic species and/or cross-linking of organic species through covalent and/or noncovalent interactions. These graphene-based hybrid materials show improved or excellent performance 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 CO₂ 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 MnO₂, ZnO and SnO₂ 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 N₂ and CO₂. Since these materials could present the capacitance due to the EDLC double layer provided by carbonaceous materials and the pseudocapacitive 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 CO₂ 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

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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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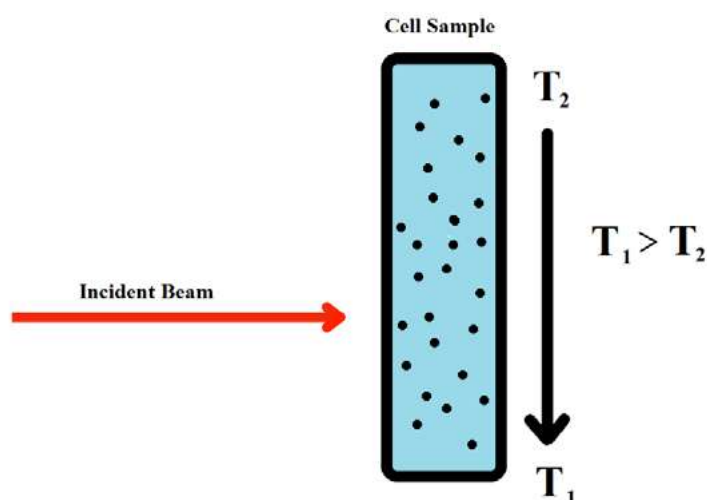


Figure 1: Schematic representation of the DLS experiment under a temperature gradient. The sample cell is subjected to a temperature difference between its base and its top.

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

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The development of solution-processable 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-processable 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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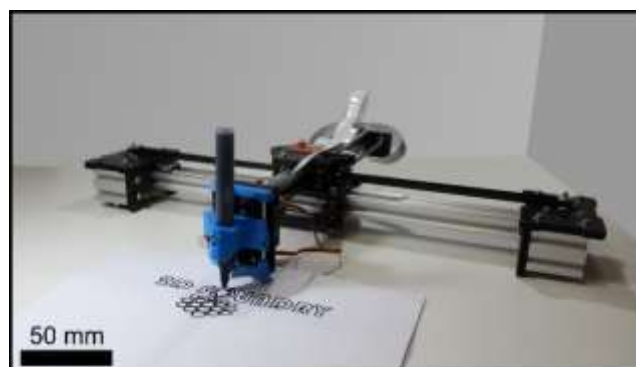


Figure 1: Digital photograph of the equipment used for printing

High-mobility MoS₂ phototransistor using biodegradable albumen dielectrics

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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 MoS₂, 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 MoS₂ transistors and photodetector devices, high carrier mobilities (up to 300 cm²/Vs) and on/off current ratios (>10⁴) 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 SiO₂-dielectrics [1]. The albumen dielectric layer is created by a basic spin coating technique and MoS₂ 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 SiO₂ 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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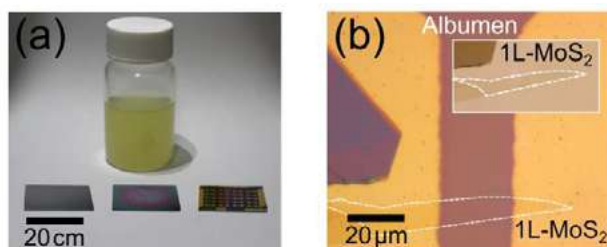


Figure 1. (a) Fabrication steps; (b) Microscope image of fabricated 1L-MoS₂ albumen transistor

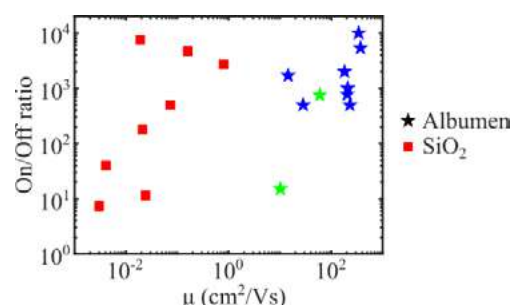


Figure 2. Mobility vs On/Off ratio. Comparison between standard SiO₂ devices and albumen devices

Electronic and ionic conduction in biomaterials based on engineered proteins

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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 $\text{Bi}_2\text{S}_3@\text{Au}$ nanocomposites

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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 $\text{Bi}_2\text{S}_3@\text{Au}$ 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 $\text{Bi}_2\text{S}_3@\text{Au}$ 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 $\text{Bi}_2\text{S}_3@\text{Au}$ nanocomposites show a larger enhancement throughout the UV-vis region possibly induced by the Au content. Finally, the anisotropic hybrid $\text{Bi}_2\text{S}_3@\text{Au}$ 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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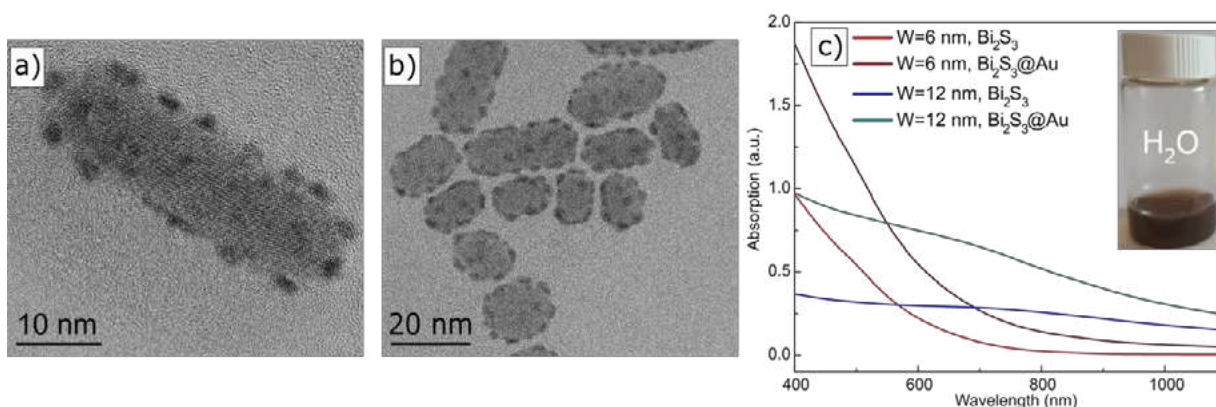


Figure 1: a) Rod-like $\text{Bi}_2\text{S}_3@\text{Au}$, b) Ellipsoidal-like $\text{Bi}_2\text{S}_3@\text{Au}$, and c) UV-vis spectra of samples with and without Au, with an image of a $\text{Bi}_2\text{S}_3@\text{Au}$ sample stable in water. W stands for the width of the nanoparticles.

Performing 3DDLS to study the dynamics of dense microgel suspensions

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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 address 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

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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 (F₆TCNNQ), with special attention to the comparison of two BTBT derivatives, namely 2,7-dioctyl-BTBT (C₈-BTBT-C₈) 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 F₆TCNNQ. The deposition of F₆TCNNQ on C₈-BTBT-C₈ 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, F₆TCNNQ on DPh-BTBT results in a planar heterostructure, without intermixing of both molecules.

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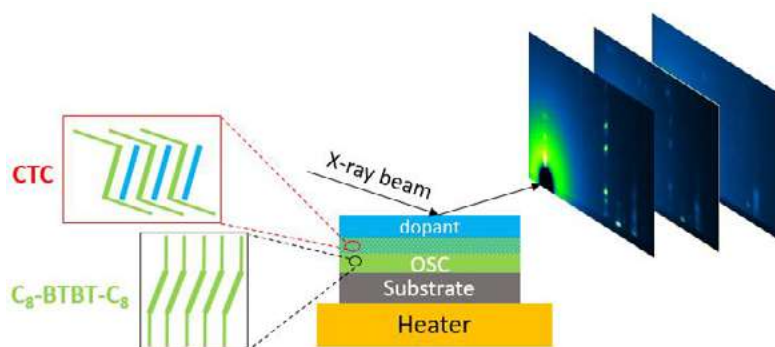


Figure 1. Sketch illustrating the structural changes upon thermal annealing for F₆TCNNQ (dopant) on C₈-BTBT-C₈ (OSC).

Percolating Superconductivity in Air-Stable Organic-Ion Intercalated MoS₂

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When doped into a certain range of charge carrier concentrations, MoS₂ 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 MoS₂. 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 MoS₂ as a platform to study the emergence and modulation of correlated electronic phases.⁴

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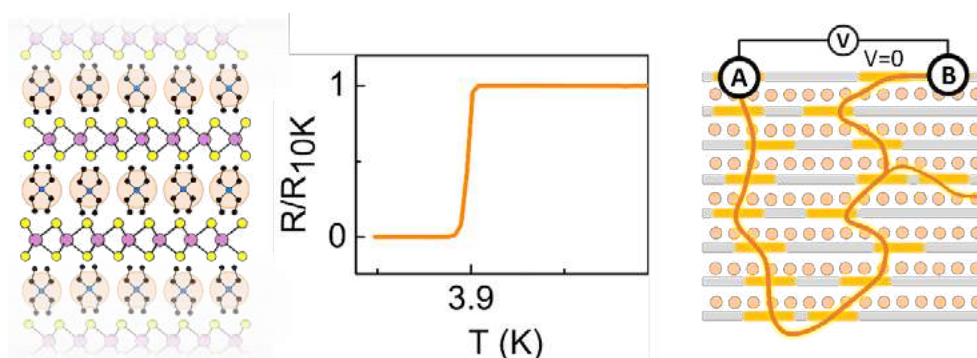


Figure 1: The intercalation of TEA⁺ cations in MoS₂ leads to the emergence of superconductivity in the bulk due to the formation of percolating path resulting from the alignment of nanoscale-sized highly-doped regions located in contiguous layers.

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

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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.

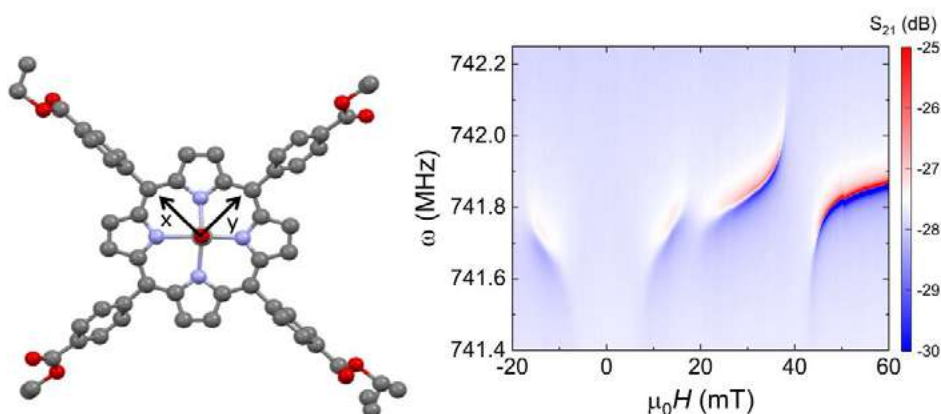


Figure 1: (Left) top view of the vanadyl porphyrin molecule, showing the vanadyl group at its centre. (Right) 2D plot of the microwave transmission of a resonator coupled to a crystal made up of these vanadyl molecules. The transitions observed at zero field and 20 mT are close to the energy minima of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

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

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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

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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 -MoO₃ [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 -MoO₃ 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

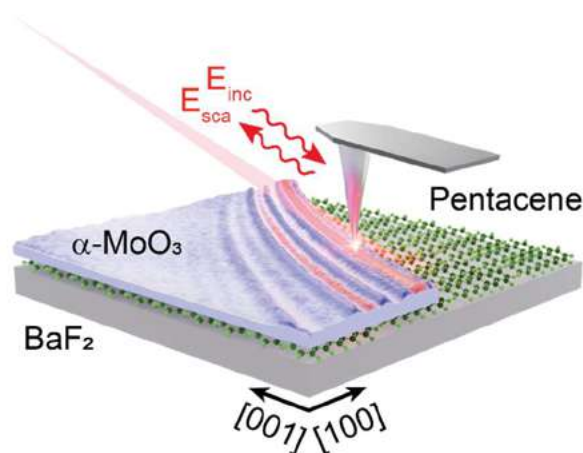


Figure 1: Schematic of the visualization by s-SNOM of strong coupling between PhPs and pentacene molecules.

Molecular electronics: insight from simulations and calculations

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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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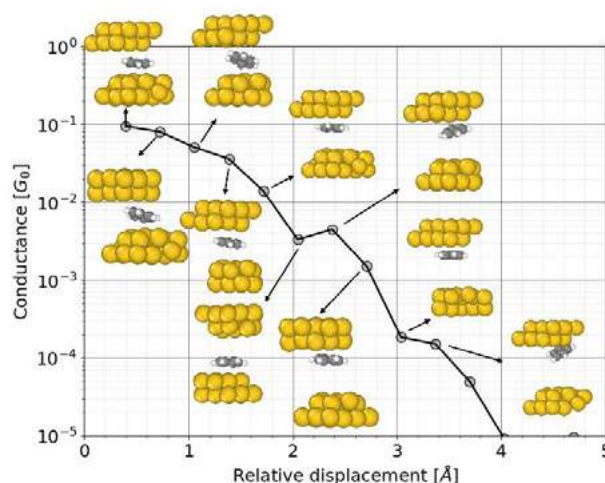


Figure 1: Electronic transport calculations versus relative displacement of the electrodes for the case of a single benzene molecule captured between gold electrodes. Inside we have illustrated the evolution of the contact simulated by CMD.

An apophatic description of spherical shells

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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

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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

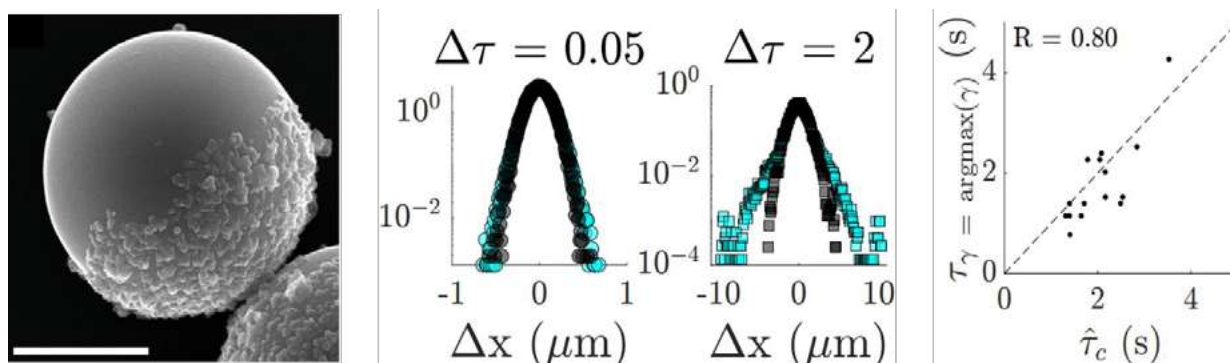


Figure 1: Influence of microswimmer motion on the dynamics of passive tracer particles. Left: HR-SEM of our synthesized, photocatalytic Janus microswimmers (scale bar 1 μm) (taken from [3]). Middle: Distribution of tracer displacements in the presence of microswimmers at different lag times ($\Delta\tau = 0.05\text{s}$, 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.

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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

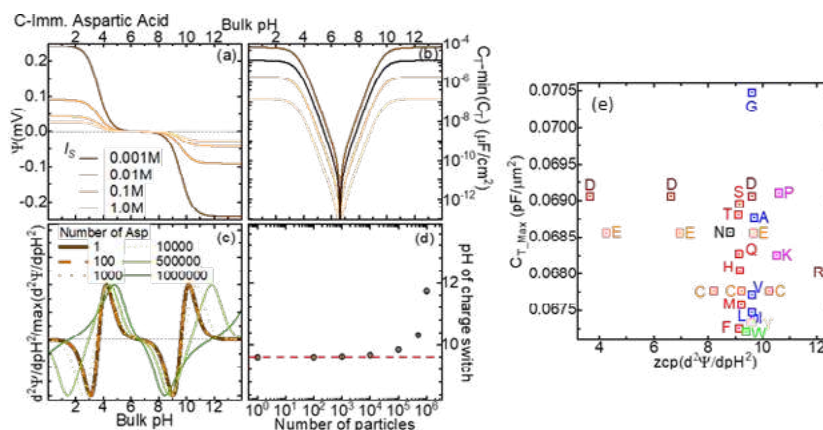


Figure 1: (a), (b) Surface potential (Ψ) and Capacitance (CT), respectively for 100 Aspartic acid molecules/ μm^2 at different Ionic strengths (IS). (c) $d^2\Psi/dpH^2$ at $IS=0.01\text{M}$ for different numbers of molecules in $1\mu\text{m}^2$. (d) crossing of the alkaline switching charge, (red line indicates the nominal value of the pK_b). (e) Calculations for fingerprints of 100 Amino Acids/ μm^2 immobilized by the C-Terminal.

The uncanny weight of granular columns

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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

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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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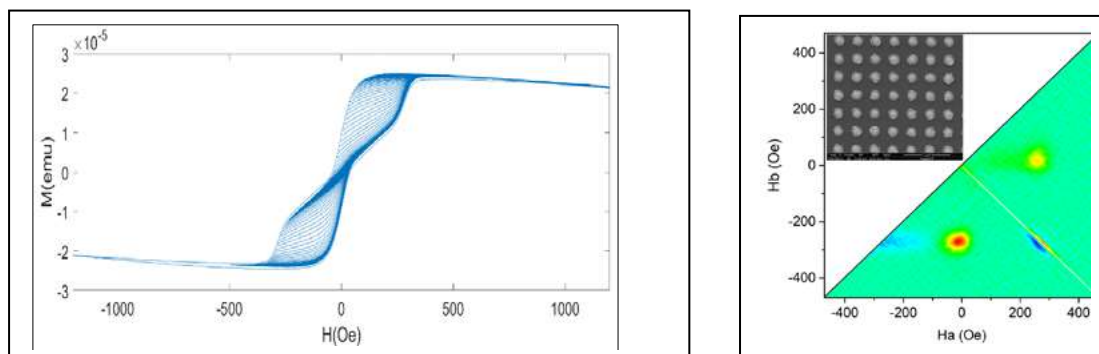


Figure 1: Example of the measurements for one of the samples, with non-interacting dots. On the right the FORC measurements taken with an AGFM, on the left the FORC distribution generated from the measurements and a SEM image of a portion of the array of nanodots.

Tunable magnetic equilibrium configurations in dipolar helices

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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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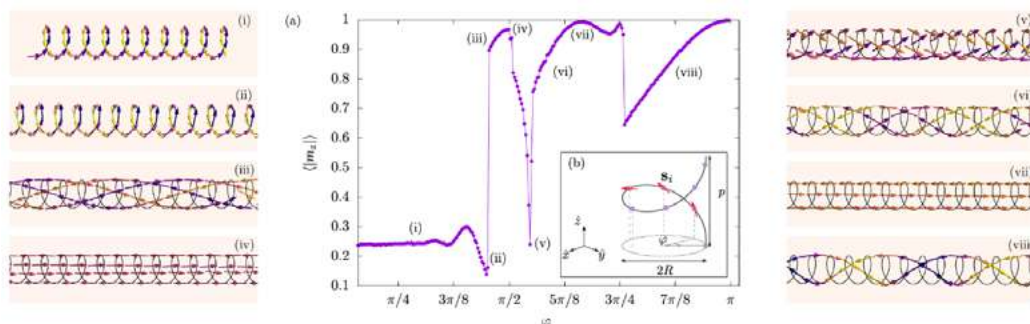


Figure: Ground states of a dipolar helix ($R=1$, $p=\pi/2$) and their staggered magnetization along the helix axis.

Strontium Titanium Chalcogenide Perovskite Photoanodes for H₂ Production

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Inorganic chalcogenide perovskites are semiconductors with general formula ABX₃, with A being a group II cation (i.e., Ca²⁺, Sr²⁺, or Ba²⁺), B a group IV transition metal (i.e., Ti⁴⁺, Zr⁴⁺, or Hf⁴⁺), and X a chalcogen anion (S²⁻ or Se²⁻) [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 Na₂SO₃ aqueous electrolytes. These results show that Sr_{1+x}TiS_{3-y} has potential interest in hydrogen production by using renewable energy resources.

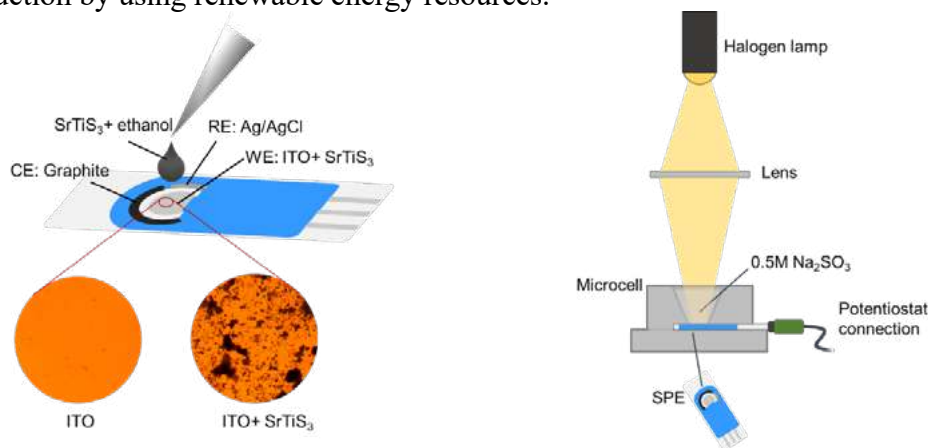


Figure 1. Schematic image of the drop coating method used to prepare the screen-printed electrodes (SPE) with our Sr_{1+x}TiS_{3-y} powders and optical microscopy images of the prepared electrodes (left panel). Scheme of the micro-electrolytic cell used to determine the photo-electrolytic properties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

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

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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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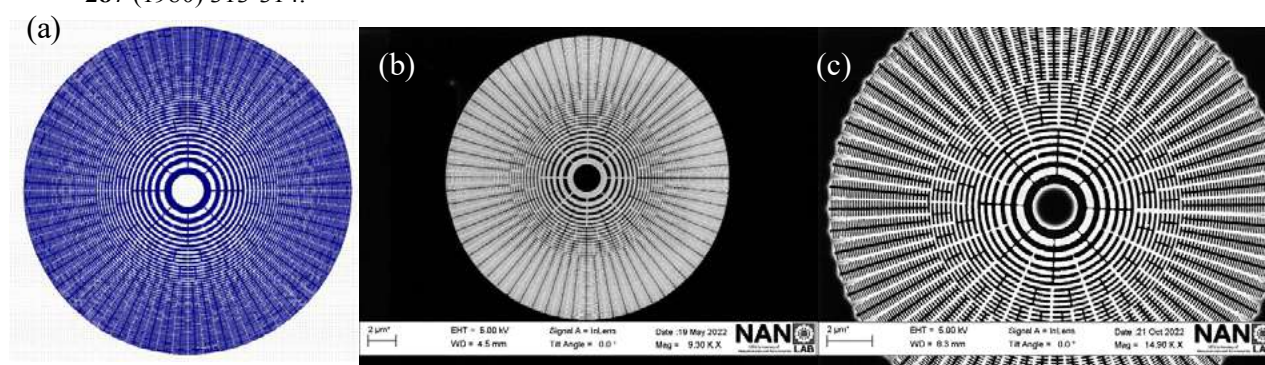


Figure 1: (a) CAD design of Fresnel zone lens, (b) Scanning electron microscope (SEM) image of FZP that has a diameter of 20 μm and an outermost zone width of 50 nm, (c) SEM overview of FZP after 15s of Silicone etching.

Plasmonic Rectification of terahertz radiation using encapsulated graphene field effect transistor

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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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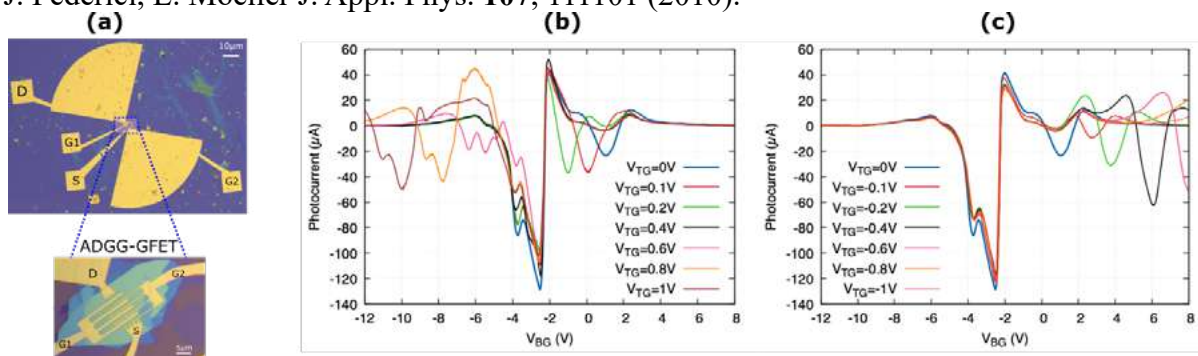


Figure 1: (a) Microscope photo of the ADGG-GFET and the measured photocurrent versus the back gate under excitation of 288GHz and at 1.7K for (b) positive top gates biases and (b) negative top gate bias

Acknowledgments

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Ga₂O₃:Cr nanowire-based optical microcavities for thermometry

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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, Cr³⁺, Gd³⁺, Er³⁺, Eu³⁺ [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 -Ga₂O₃: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 -Ga₂O₃:Cr nanocavities is monitored: the characteristic R-lines of Cr³⁺ 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

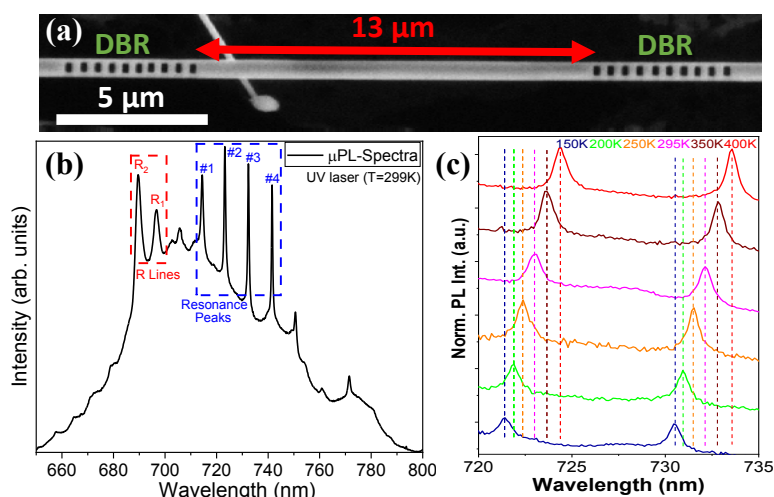


Figure 1: (a) SEM image of the optical cavity created in a β -Ga₂O₃:Cr nanowire, (b) local micro-photoluminescence spectrum for 299 K, (c) FP peak positions dependence on temperature.

Resonant tunneling energy harvesters: improving performance via quantum interference

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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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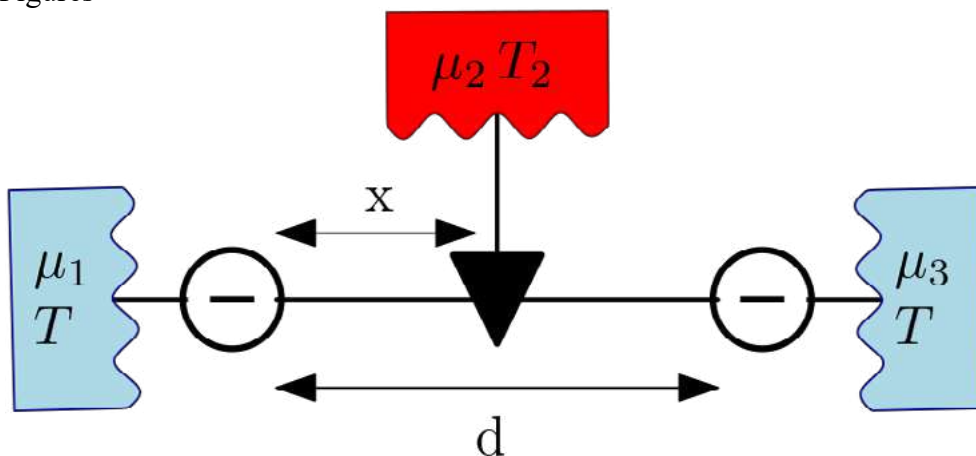


Figure 1: Sketch of the three-terminal device.

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

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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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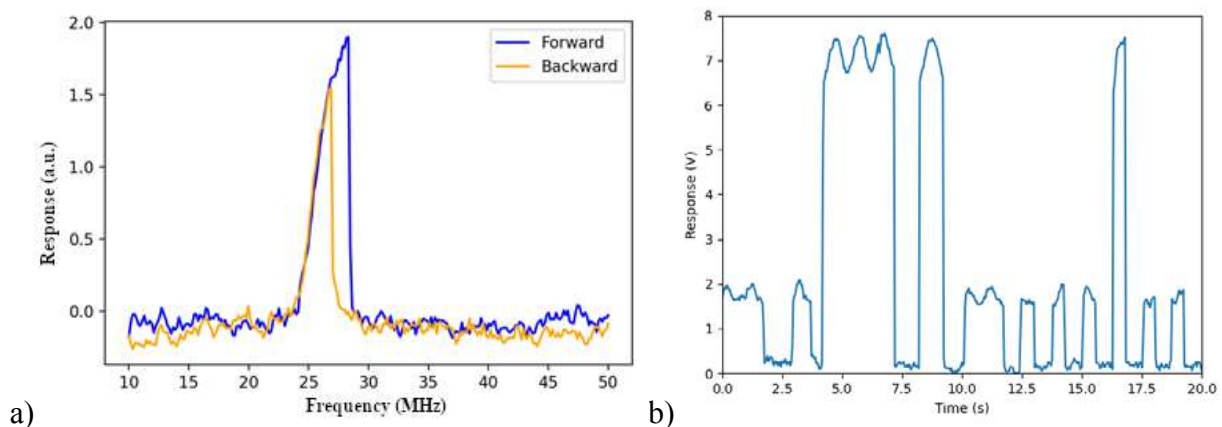


Figure 1: a) Spectral response of one of our MoS_2 resonators showing a strong nonlinear behavior. b) Electrooptical response of the system under a slow-varying FM signal with a center frequency of 27.4 MHz and 500 kHz deviation.

Floquet theory of electronic stopping of nuclear projectiles in solids

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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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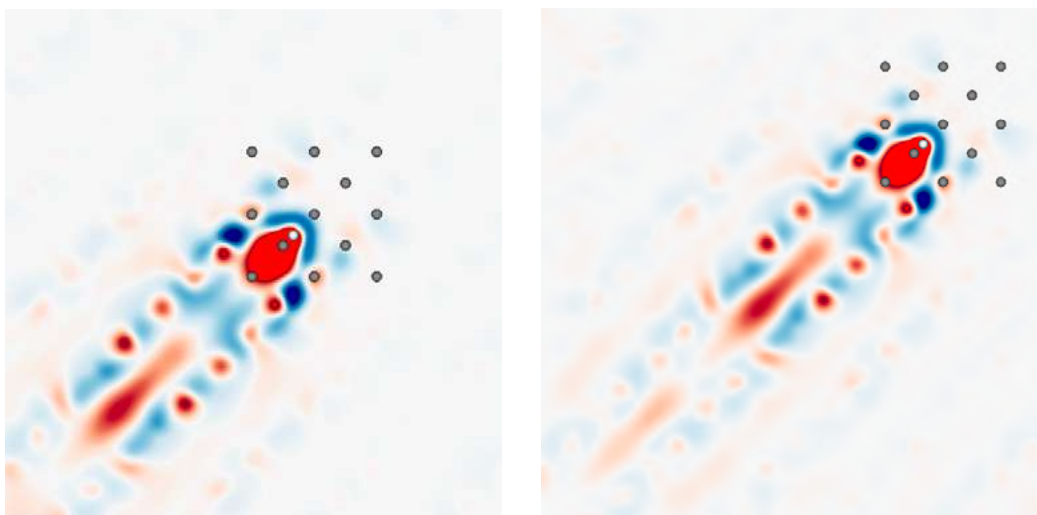


Figure 1: Electron deformation density in real space at equivalent projectile positions in consecutive diamond unit cells (left and right panels) along the trajectory for a proton moving at $v = 1$ a.u. along the $[110]$ direction, depicted in the (001) plane containing the projectile. Color scale: from -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

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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 systems¹, 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 Nd³⁺ 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 μ s 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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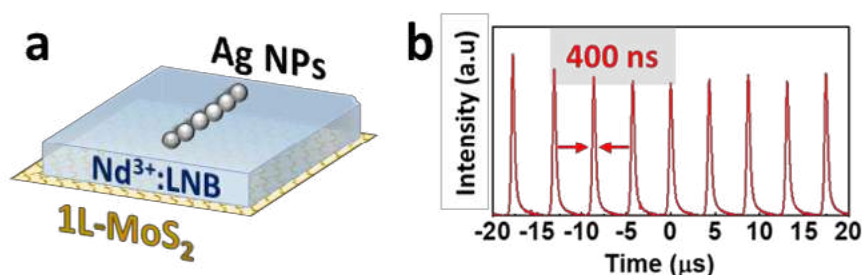


Figure 1: a) Schematics of the monolithic architecture for pulsed nanolasing. The hybrid system includes: Nd³⁺-doped LiNbO₃ as a gain media, plasmonic Ag nanoparticle chains for sub-wavelength spatial confinement, and 1-layer MoS₂ for temporal confinement of laser radiation. b) Temporal evolution of laser emission.

Scalable and low-cost fabrication of flexible WS₂ photodetectors on polycarbonate.

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We present a low-cost and easy-to-implement technique to fabricate large-area WS₂ 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 WS₂ 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 μ W) and response time (down to ~70 μ s) and a detectivity value of 10⁸ Jones. We found that the devices perform very reversibly upon several illumination and straining cycles and we found a moderate device-to-device variation.

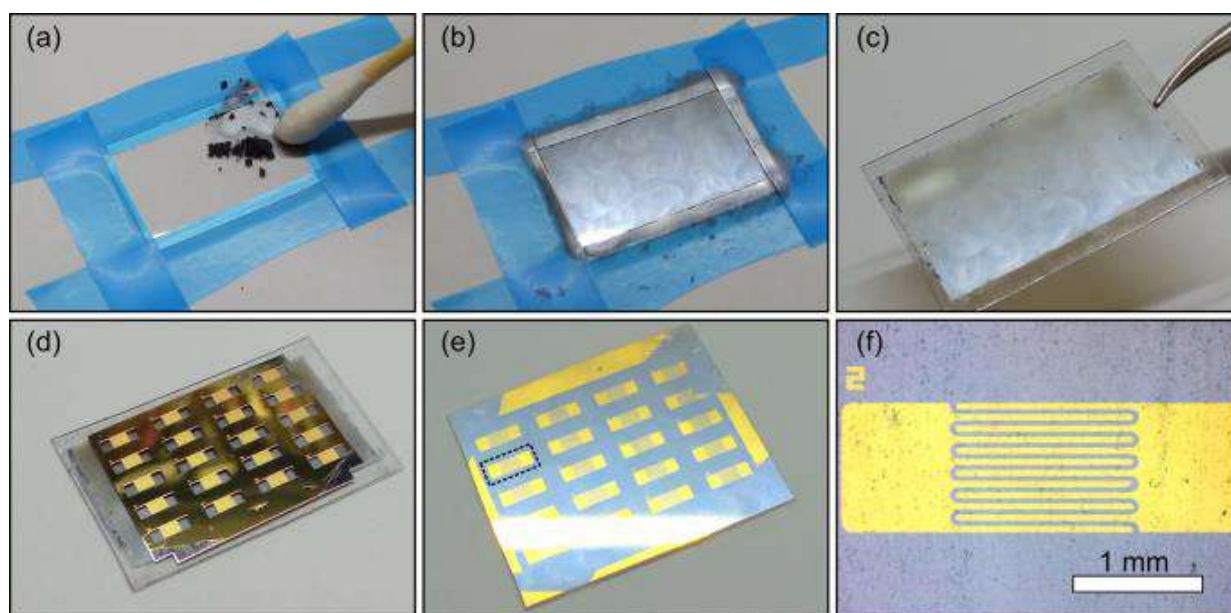


Figure: **a** Fine WS₂ powder is rubbed against the surface of a polycarbonate substrate with a cotton swab. **b, c** Pictures of the WS₂ film on polycarbonate after deposition. **d** A shadow mask is placed onto the surface of the film. **e** Picture of a polycarbonate chip after the evaporation of 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

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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 150° 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

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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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Figures

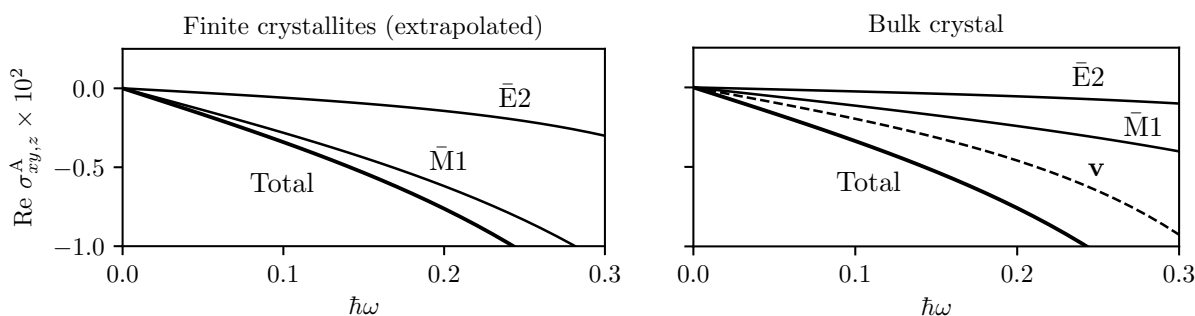


Figure 1: Decomposition of the spatially-dispersive conductivity tensor into three types of origin-independent contributions: intrinsic magnetic dipole (M1), intrinsic electric-quadrupole (E2) and band-dispersion (v). The latter is only present in the bulk calculations on the right, and it must be included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

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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

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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 BaB₂O₄ (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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Figures

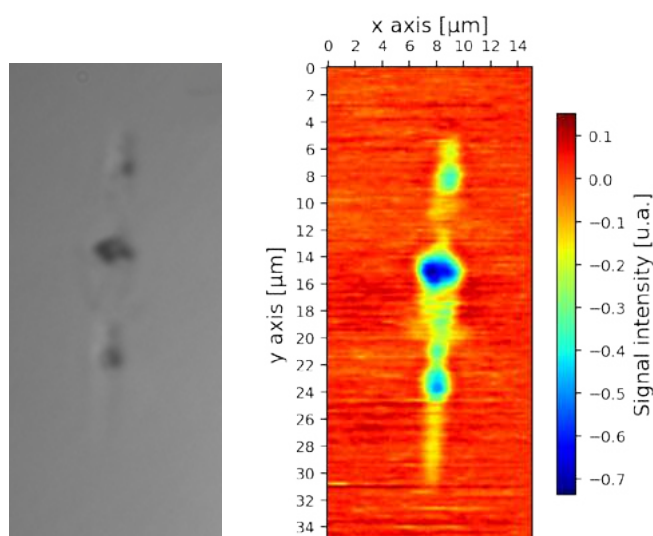


Figure 1: Example of the obtained results. Left; Optical image of a damage track induced at 118 μm below the surface of a BBO crystal with 60 fs, 60 mW pulses. Right; Corresponding SHM map of the damage track.

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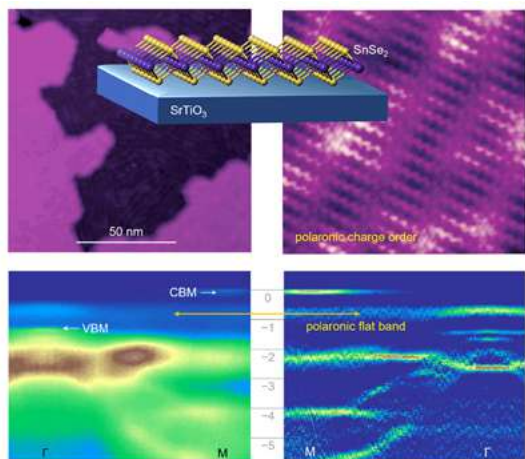


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Interfacial Polarons in van der Waals Heterojunction of Monolayer SnSe₂ on SrTiO₃ (001). STM and ARPES measurements of the monolayer SnSe₂ epitaxially grown on Nb-doped STO(001). Aidi Zhao and Bing Wang
Nano Letters 2020 20 (11), 8067-8073
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Emergence of Floquet band structure in Dirac Hamiltonians by short pulse irradiation

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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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Figures

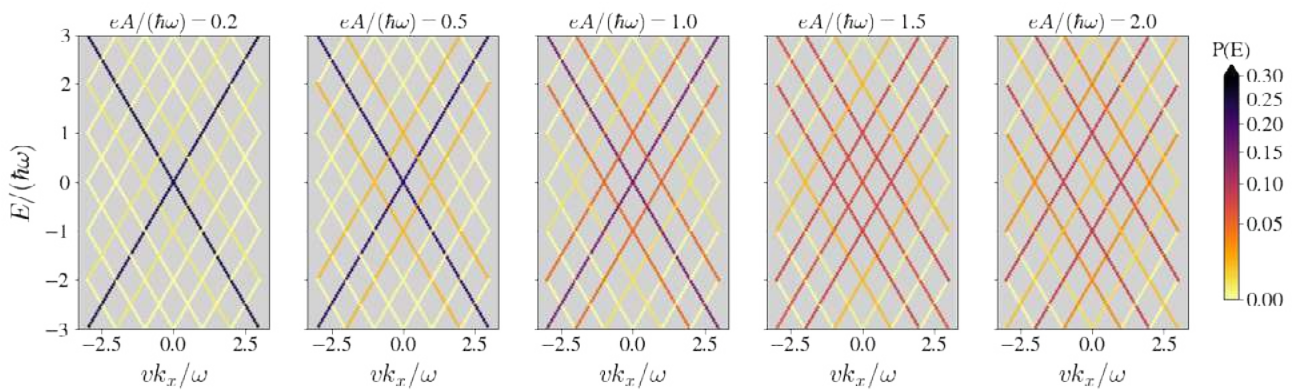


Figure 1: Spectral density projected onto the Floquet replicas for a Dirac Hamiltonian and a linearly polarized driving.

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

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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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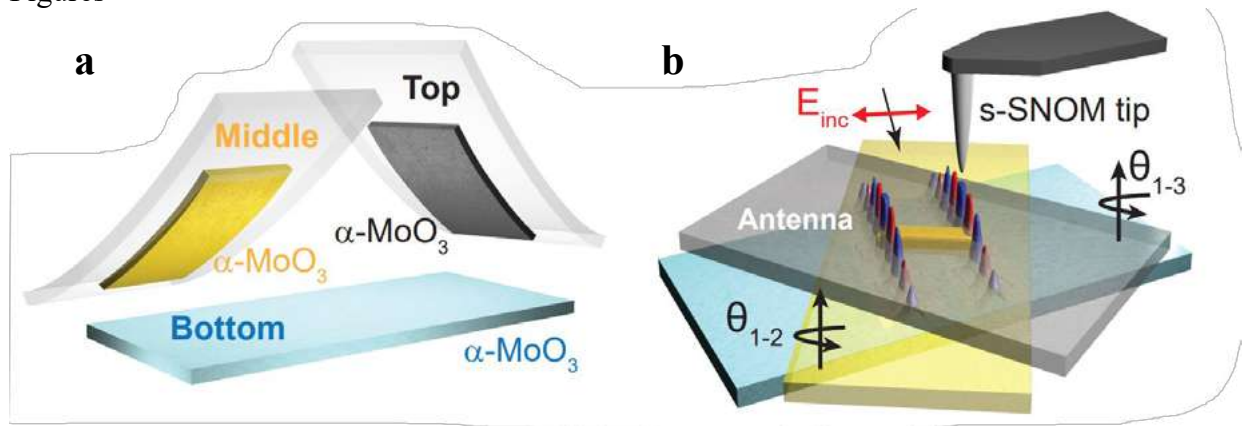


Figure 1: (a) Schematic of a twisted biaxial system made of three α -MoO₃ layers. (b) Schematic of the excitation of polaritons in a twisted biaxial system by a scattering-type scanning near-field optical microscopy (s-SNOM).

Supression of superradiance by magnetic correlations

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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 1 K, the system is in an 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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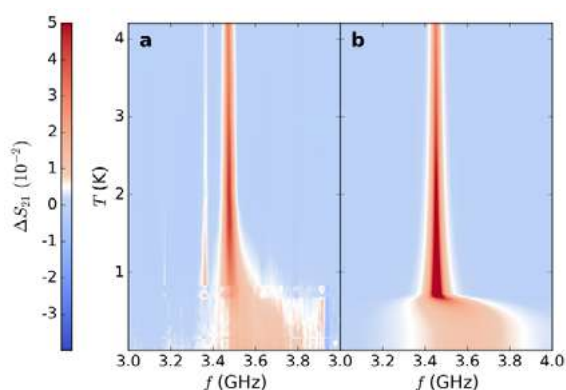


Figure 1: Suppression of superradiance as low temperatures onset magnetic correlations. (a) Experimental transmission and its theoretical simulation (b).

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

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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 Nd³⁺ 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 Nd³⁺ 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 Nd³⁺ ions emit.

The results are explained considering the near field coupling of the Nd³⁺ 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 Nd³⁺ 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

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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 $\mathbf{k} \cdot \mathbf{p}$ 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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Quantum chaos in the Bose-Hubbard model

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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 $n \leq 1$ [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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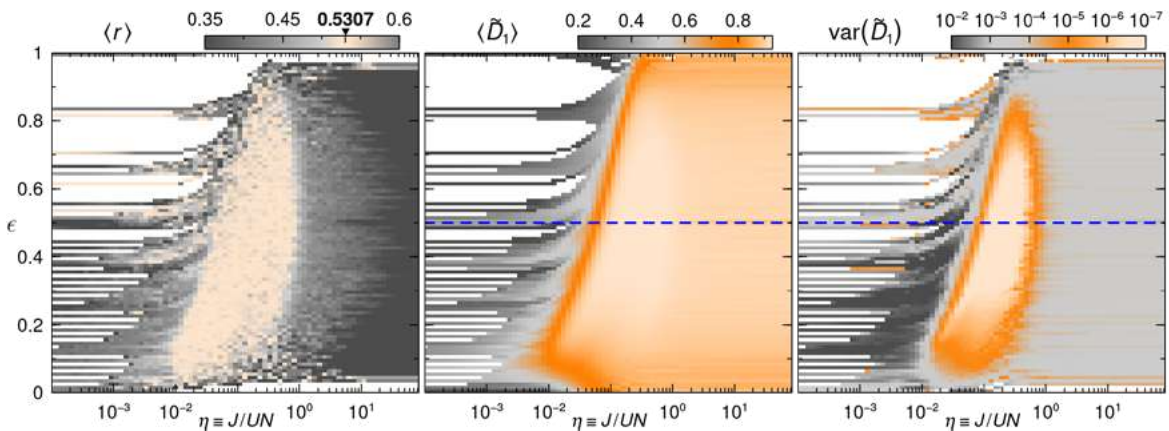


Figure 1: Chaotic phase of the Bose-Hubbard Hamiltonian exposed by spectral statistics (left), and eigenvector features characterized by generalized fractal dimensions (middle and right), for an irreducible Hilbert subspace of a system of 12 bosons in 12 spatial modes.

Hyperbolic light interacting with molecules

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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, MoO₃, V₂O₅ 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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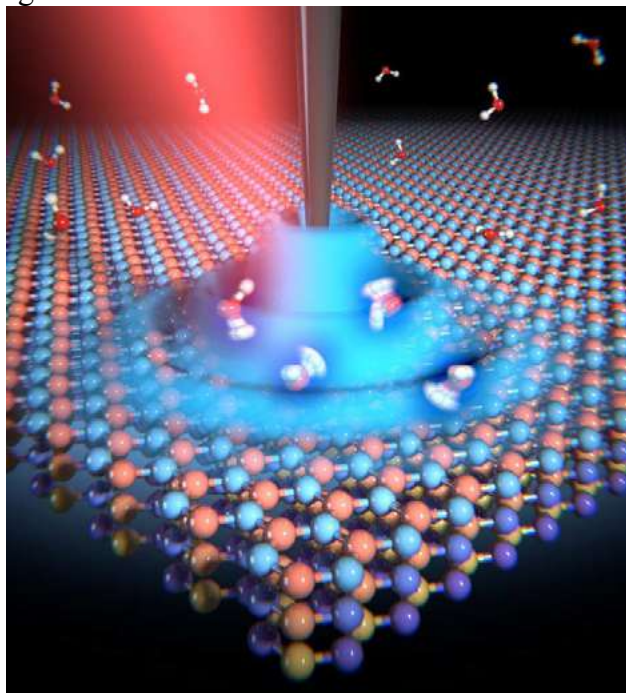


Figure 1: An artistic image of a phonon polariton in h-BN interacting with molecular vibrational resonances. The vertical rod represents the AFM tip of a near-field optical microscope, probing the interaction.

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

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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.

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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

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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

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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

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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

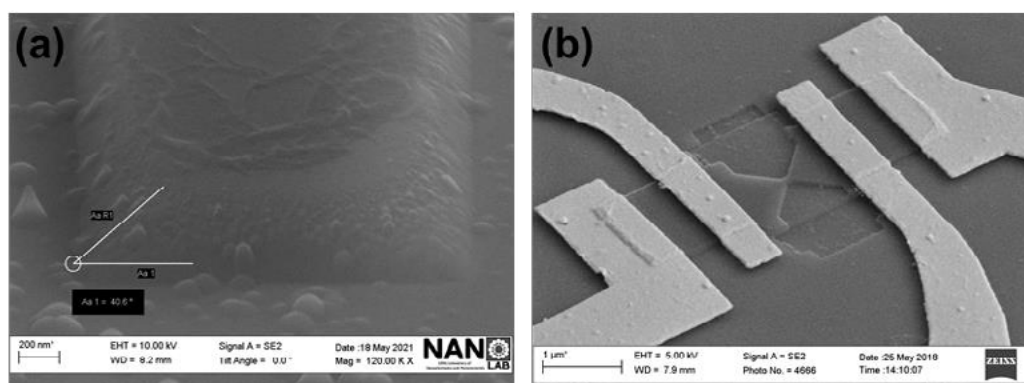


Figure 1: (a) Etching of a (thick) h-BN at 10 °C. (b) Constriction of 100 nm in encapsulated graphene with etching at -110 °C.

Topological states in finite graphene nanoribbons

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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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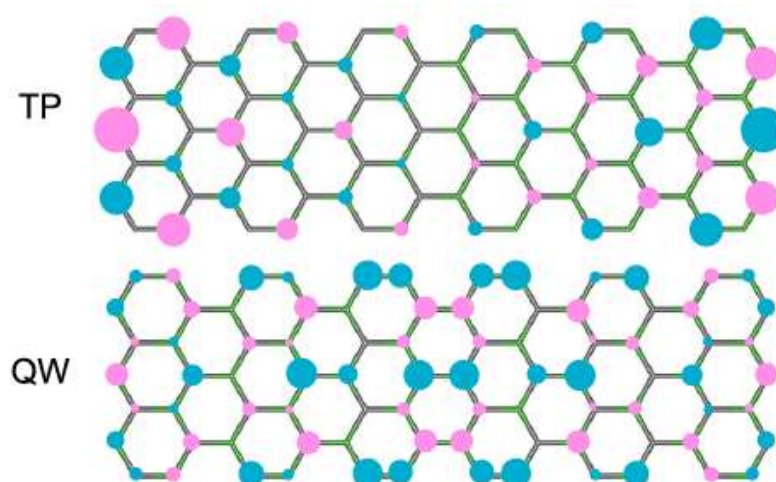


Figure 1: Wave function distribution for the two first occupied states corresponding to an Armchair Graphene Nanoribbon with seven atoms of width. Blue and pink indicate positive and negative amplitudes, respectively.

Scanning Tunneling Spectroscopy in topological Dirac semimetal ZrTe₅

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ZrTe₅ 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 ZrTe₅ to display Quantum Hall Effect among other notable phenomena with interesting application for the development of electronic device applications [3]. The nature of ZrTe₅ 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 ZrTe₅ 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 ZrTe₅ 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 WTe₂ visualized by Scanning Tunneling Microscopy

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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 WTe₂. 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 WTe₂. 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

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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 to 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

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The bulk photovoltaic effect (BPVE) is a phenomenon that consists in the generation of a DC current in a material under illumination 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) solving the time-dynamical equations for the density matrix including 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, including 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 $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ / SrIrO_3 bilayers

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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 $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ 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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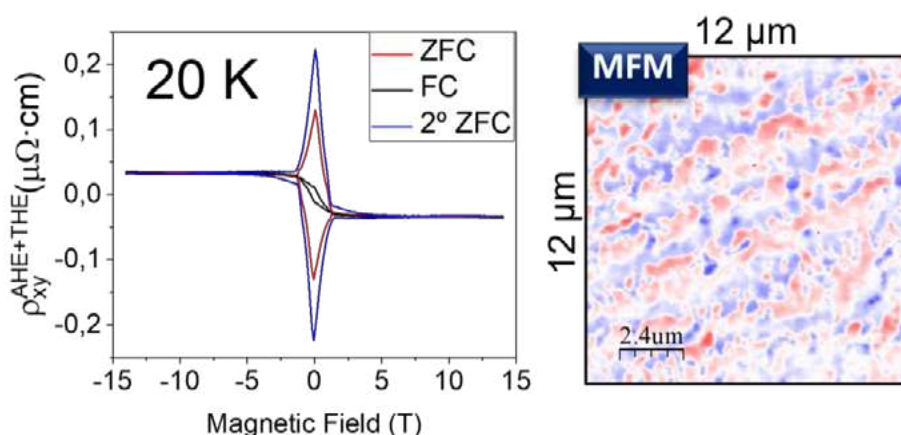


Figure 1: Left panel. Anomalous Hall effect measured at 20 K after field cooling (FC) (black line) and zero field cooling (ZFC) (red and blue lines). Right panel. MFM image at 17 K after ZFC.

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

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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 $\lambda_p/4.5=\lambda_0/50$ (λ_p is the polariton wavelength and λ_0 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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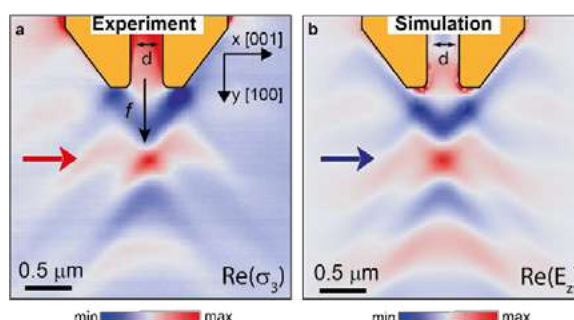


Fig. 1 Nanofocusing of PhPs along the surface of a α -MoO₃ flake into deep-subwavelength focal spots.

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

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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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Figures

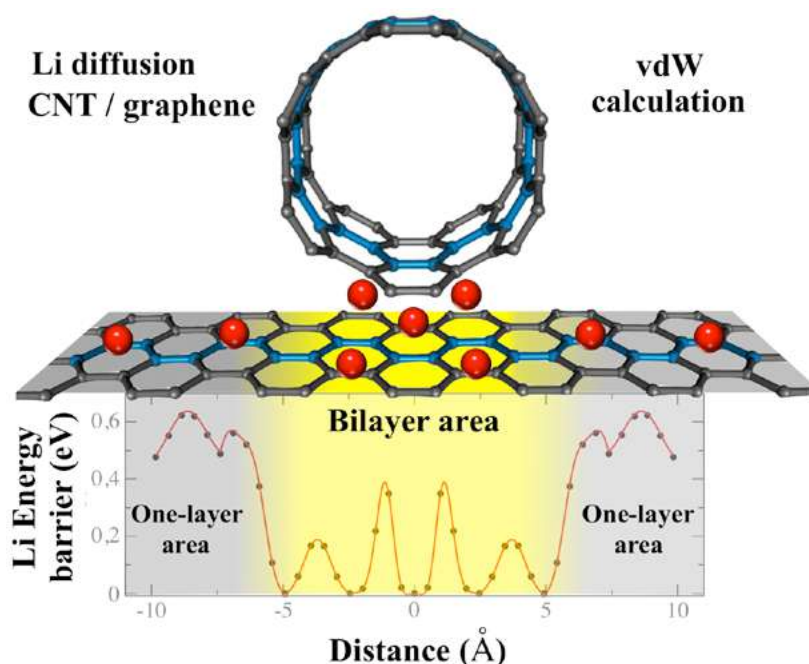


Figure 1: Energy barriers of Li along different paths over grafene / CNT heterostructure by NEB VASP calculation.

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

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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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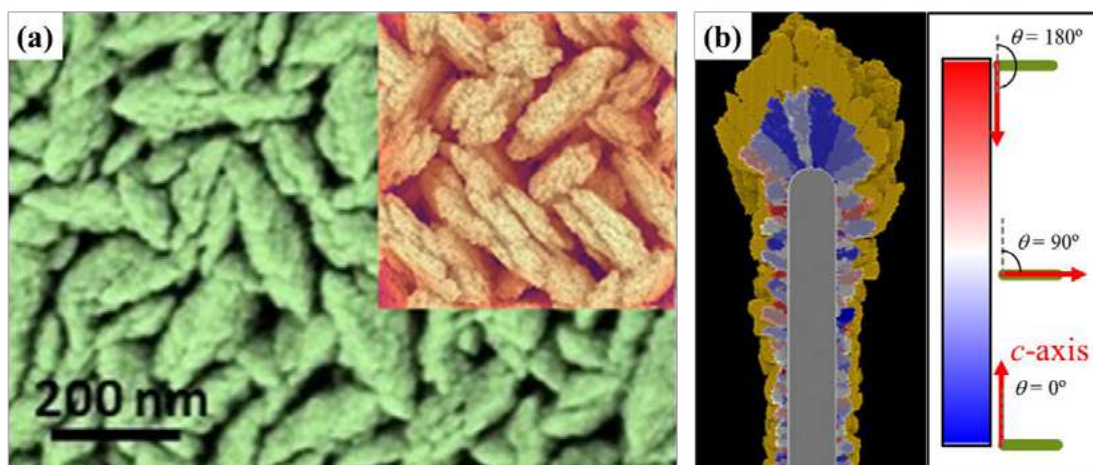


Figure 1: (a) Top-view Scanning Electron Microscopy micrograph of a wurtzite-type ZnO film with nanocolumnar morphology fabricated by PECVD on Si substrates at RT conditions under oxygen plasma and growth rate of 10 nm/min. The inset is the simulated thin-film morphology obtained by assuming similar growth conditions. (b) Longitudinal cut of a simulated ONW@ZnO@SiO₂ 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

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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 within 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

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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

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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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Figures

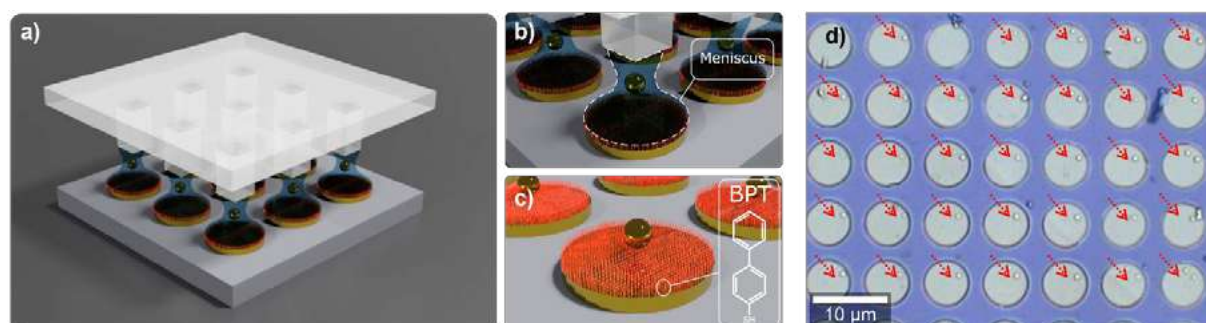


Figure 1. a) Schematic parallel stamp-assisted printing method. b) Meniscus formation between the stamp protrusion and sample. c) BPT Functionalized lithographed Au sample with NP attached. d) Optical image of a Au/BPT disk array after single-step NP transfer. Red arrows show NP positioning.

Interaction-driven Circular Dichroism through absorption modes in Triskelia Nanostructures

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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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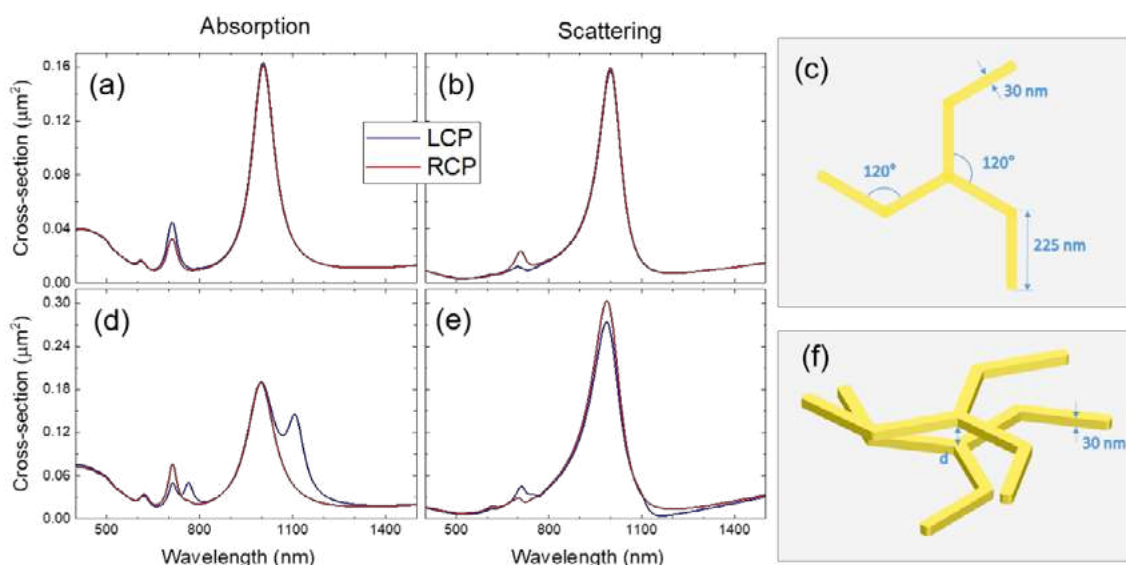


Figure 1. Absorption (a) and scattering (b) cross-section spectra for a single triskelion, and (d) and (e) two triskelia with a relative rotation angle of 30° and 30 nm of separation. Right panels (c) and (f) show schematic representations of a single triskelion and two triskelia, respectively.

Vortex lattice at high magnetic fields and charge density wave in $\text{KCaFe}_4\text{As}_4$ and $\text{CaK}(\text{Fe}_{0.988}\text{Mn}_{0.012})$

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The 1144 $\text{CaKFe}_4\text{As}_4$ compound is a pnictide superconducting material showing optimal superconducting critical temperature with T_c 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 T_c 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 $\text{CaKFe}_4\text{As}_4$ 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 $\text{CaKFe}_4\text{As}_4$. 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 $\text{CaKFe}_4\text{As}_4$ 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 $\sqrt{2}a_0 \times \sqrt{2}a_0$ where a_0 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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Inducing strain in hybrid van der Waals heterostructures based on spin-crossover layers and two-dimensional materials.

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Van der Waals heterostructures (vdWHs) provide the possibility of engineering new materials with emergent functionalities that are not accessible in another way. These heterostructures are formed by assembling layers of different materials used as building blocks. Beyond inorganic 2D crystals, layered molecular materials remain still rather unexplored. In this work, the family of van der Waals heterostructures is enlarged by introducing a molecular building block able to produce strain: the spin-crossover (SCO). In these metal-organic materials, a spin transition can be induced by applying external stimuli. In particular, smart vdWHs are prepared in which the electronic and optical properties of the 2D material (graphene, WSe₂) are switched by the strain caused by the spin transition. These hybrid vdWHs represent the deterministic incorporation of bistable molecular layers with other 2D crystals in the emergent fields of straintronics and band engineering in low-dimensional materials.

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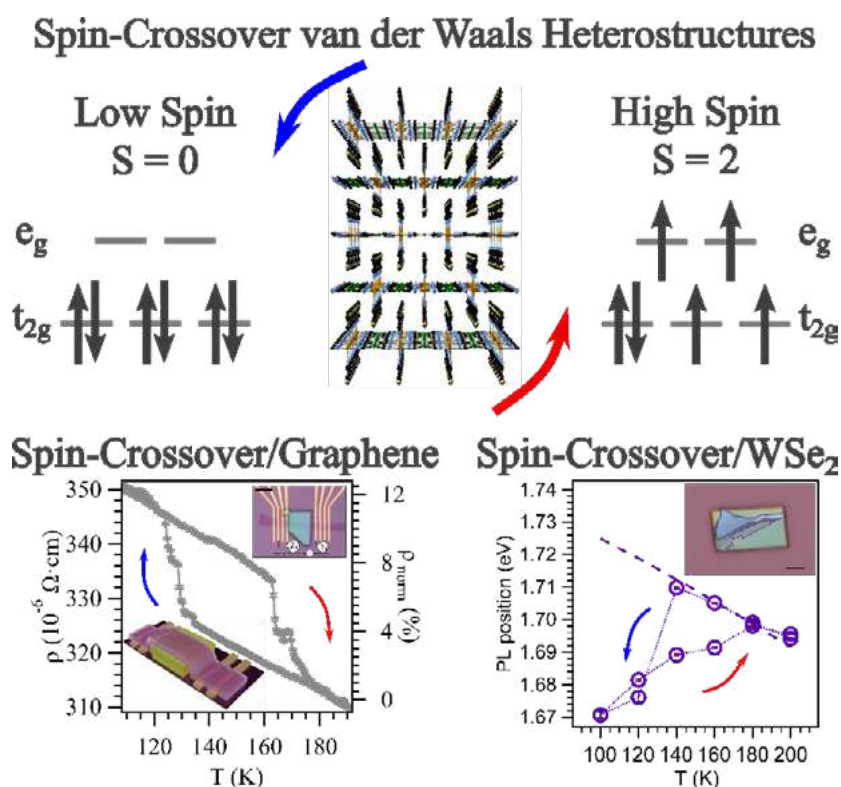


Figure 1: Upper figure: Scheme of the spin-crossover phenomenon for a d^6 (Fe^{2+}) metal complex. Bottom left: Thermal dependence of the resistivity for a vdWH. Bottom right: Thermal dependence of the PL position for the vdWH and a reference WSe₂ monolayer.

Operando GIWAXS and HAXPES on Blue Perovskite Light Emitting Diodes

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Metal Halide perovskites are promising candidates for next generation displays. Advances in the field have us Light Emitting Diodes (LEDs) that have external quantum efficiency above 20%¹ for green and red colours while blue is still far behind such values. Much effort has been put into understanding perovskite as a material, learning its favourable optoelectronic properties and discovering how to shape the semiconductor to our specific needs. However, our depth of knowledge fails when we investigate the same perovskite material in the context of a working device. Here we show results of our study where we conduct *operando* Grazing Incidence Wide Angle Xray Scattering (GIWAXS) measurements and Hard Xray Photoemission Spectroscopy (HAXPES) on our blue perovskite LEDs. Simultaneously we collect the electroluminescence spectra and current voltage characteristics of the device. The combination of these techniques allows us to probe the active material during operation and record live both structural and chemical changes that occur inside the perovskite device.

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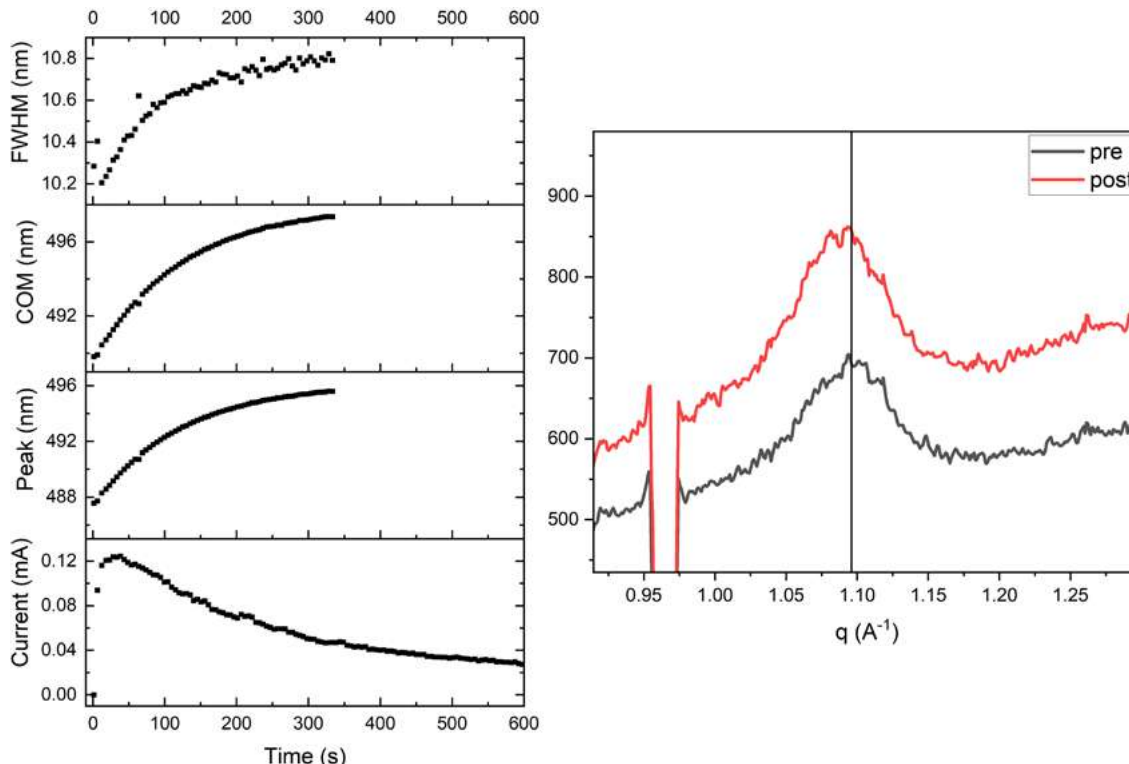


Figure 1: Left: evolution of the electroluminescence spectra and JV characteristic over time of a sky blue perovskite LED. Right: GIWAXS scan of the main perovskite peak of the same perovskite LED before and after electrical bias highlighting the peak shift that occurs.



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Ferromagnetism on a single atom-thick 2D-metal-organic framework

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Single layer metal-organic frameworks (MOFs) grown on metallic substrates have been candidates for 2D-Ferromagnetism (FM) due to the chemical control, tunability of the organic linkers and the rich self-assembled architectures achieved. Despite many attempts, FM in 2D-MOFs had never been observed. In this work we show cooperative ferromagnetism (FM) in an atom thick two-dimensional metal- organic framework. We study a 2D-MOF consisting of Fe atom centers and 9,10-dicyanoanthracene (DCA) molecular linkers forming a mixed honeycomb-kagome lattice on Au(111), so called Fe+DCA/Au(111). The lattice is formed by sequential deposition of DCA and Fe atoms on Au(111) with Fe:DCA relation of 3:2. Large, monodomain network islands are generated. LEED patterns show a hexagonal network, with nn Fe distance = 1.15 nm. By means of an experimental approach consisting of STM and STS, LEED, XAS and XMCD, as well as state-of-the-art first-principles calculations, we show that 2D-FM takes place in Fe-DCA/Au(111) below $T_c = 35$ K, driven by exchange interactions through the molecular linkers. The system exhibits a square hysteresis loop and coercive fields over 2T, with huge remanence and perpendicular anisotropy.

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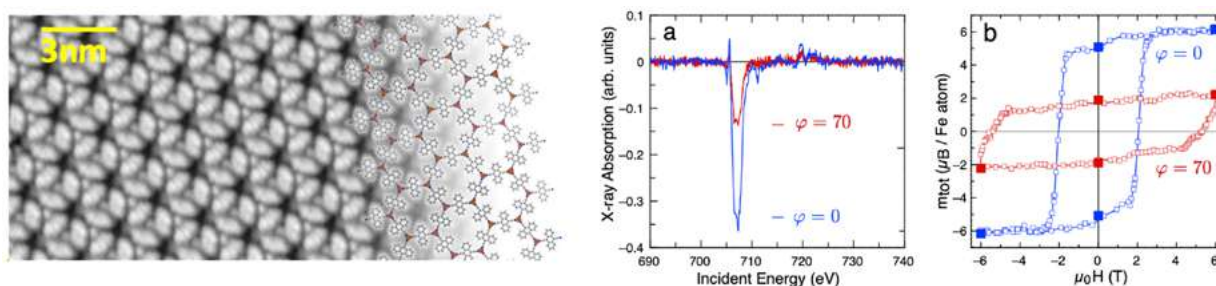


Figure 1: Left: STM image (20 pA; -1 V) of the 2D-MHK lattice with a model of the MOF structure overlaid with the molecules forming a kagome substructure and the Fe adatoms a honeycomb sublattice. Right a) $L_{2,3}$ Fe-edge XMCD spectra acquired for normal (0) and grazing (70) incidence angle. Right b) Hysteresis loop obtained at the L_3 edge of Fe at normal (green) and grazing (red) incidence.

Synthesis and characterization of perovskite thin films by polymer-assisted deposition for spintronic application

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Lanthanum strontium manganite ($\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$) is a perovskite oxide with a huge appeal because of its wide variety of electronic and magnetic properties, such as colossal magnetoresistance, half-metallicity, and metal-insulator transitions [1], which can be tuned by Sr doping level, as it is responsible for Mn ions valence [2]. Epitaxial $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ thin films with high-quality, well-oriented, with minimal structural and chemical imperfections are desired. The polymer-assisted deposition (PAD) technique was chosen among the different grown methods, as it is a promising methodology with environmentally friendly, low-cost scalability and stoichiometric versatility [3].

Taking advantage of the PAD's stoichiometric versatility, epitaxial oxide $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ thin films, with $0.3 \leq x \leq 0.65$, were grown on top of single crystalline (001)- SrTiO_3 substrates. Flat and fully strained $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) epitaxial thin films could be obtained with the expected ferromagnetic behaviour ($T_c = 340$ K). In addition to the characteristic resonant peaks that these films displayed when characterized by ferromagnetic resonance, LSMO films also evidenced a spin-pumping effect when a Pt film was deposited on top of it. Thus, PAD demonstrated its efficiency in growing high quality LSMO epitaxial films for spintronic applications.

$\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ thin films with $x \geq 0.5$ were grown to use its A-type antiferromagnetic (AF) behaviour to improve the spin injection from a ferromagnet into a normal metal [4]. However, it was necessary to reach a doping level of 0.65 to get the expected $\text{Mn}^{3+}:\text{Mn}^{4+}$ ratio according to XAS study. $\text{La}_{0.35}\text{Sr}_{0.65}\text{MnO}_3$ thin films should have ferromagnetic ordering planes, which are coupled antiferromagnetically, thus resulting in transport anisotropy along these films.

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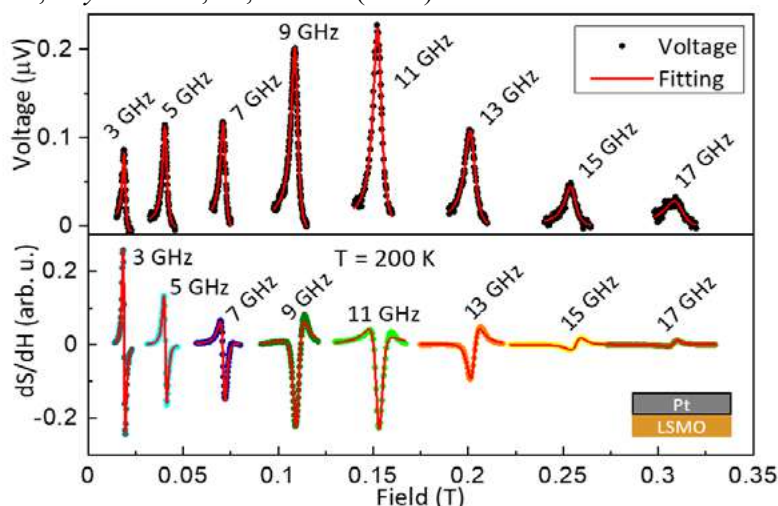


Figure 1: Inverse Spin Hall voltage signal and FMR spectra as a function of applied magnetic field measured at 200 K for different frequencies for the Pt/LSMO/STO system.

Field-induced spin wave reflection by domain walls in synthetic antiferromagnets

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Synthetic antiferromagnets (SAF) are composed by two magnetic layers separated by a nonmagnetic spacer that produces an antiferromagnetic coupling (AF) between them. They are being investigated thoroughly these days because they present remarkable features, such as suppression of skyrmion Hall effect [1] or high speed domain wall propagation [2]. From the point of view of magnonics they are also interesting because in the presence of a magnetic field they present two modes and they can be tuned by the strength of the AF coupling [3].

In this work we use micromagnetic simulations to investigate the interaction between spin waves (SWs) and domain walls (DWs) in SAFs. The DW is initially located at the center of the nanostripe and the SWs are excited at the left edge by means of a linearly polarized oscillating field mimicking the Oersted field generated by an AC current (fig. 1a). When an out-of-plane field of 300 mT or above is applied, the DW reflects the SWs very efficiently (fig. 1b). This effect is attributed to the sizable DW stretching exerted by the field, which tends to displace the DW in each layer in opposite directions. The field breaks the AF component at the DW and it acts as a barrier for the AF magnons. We have systematically evaluated SW reflection and DW displacement as a function of both the applied field and the excitation frequency finding a large correlation between them. This is explained considering that the magnons transfer linear momentum to the DW when they are reflected, leading to the DW displacement away from the SW source. Regarding the frequency dependence, the external field breaks the symmetry between the two AF modes and it is found that the lower branch, dominated by the layer in which the magnetization is antiparallel to the field, is largely responsible for the observed effect. Magnons from the upper branch, on the other hand, cross the DW without apparent reflection and they transfer their angular momentum to the DW, which leads to its displacement along the magnon flow, although their effect on the net displacement is very small as compared to the dominating effect from the lower branch. This is confirmed when each of the two modes is selectively excited using circularly polarized rf field.

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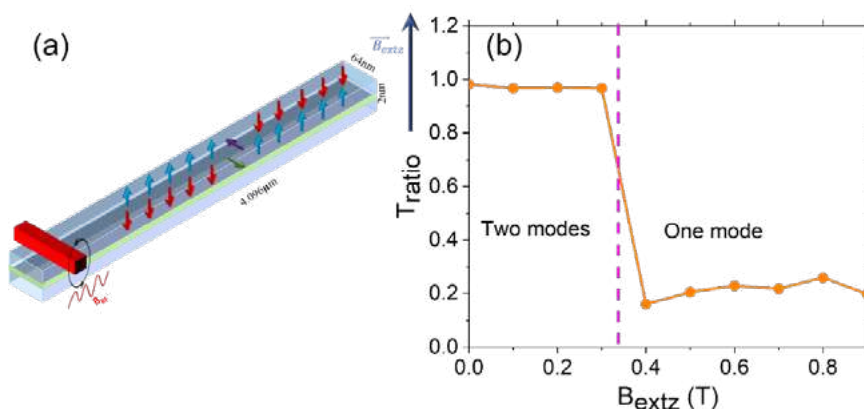


Figure 1: (a) Schematic representation of excitation of spin waves in a SAF that has a DW. (b) Spin waves transmission as a function of the applied field for an excitation frequency of 50 GHz.

Dynamics and reversible control of the vortex Bloch point domain wall in short cylindrical magnetic nanowires

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Low dissipation switching of nanomagnets is one of the main challenges in the development of future magnetic memories. We numerically investigate the evolution of the static and dynamic spin wave (SW) magnetization in short (50-400 nm length and 120 nm diameter) cylindrical ferromagnetic nanowires, where competing single vortex (SV) and vortex domain wall with a Bloch point (BP-DW) magnetization configurations could be formed. For a limited length range (between 150 and 300 nm) we demonstrate a reversible microwave field induced (forward) and opposite spin currents (backwards) transitions between the topologically different SV and BP states. By tuning the nanowire length, excitation frequency, microwave pulse duration and the spin current values we show that the optimum (low power) manipulation of the BP-DW could be reached by a microwave excitation tuned to the main SW mode and for nanowire lengths around 230-250 nm, where single vortex domain wall magnetization reversal via nucleation and propagation of SV-DW takes place. Our findings open a new pathway for the creation of unforeseen topological magnetic memories.

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Figures

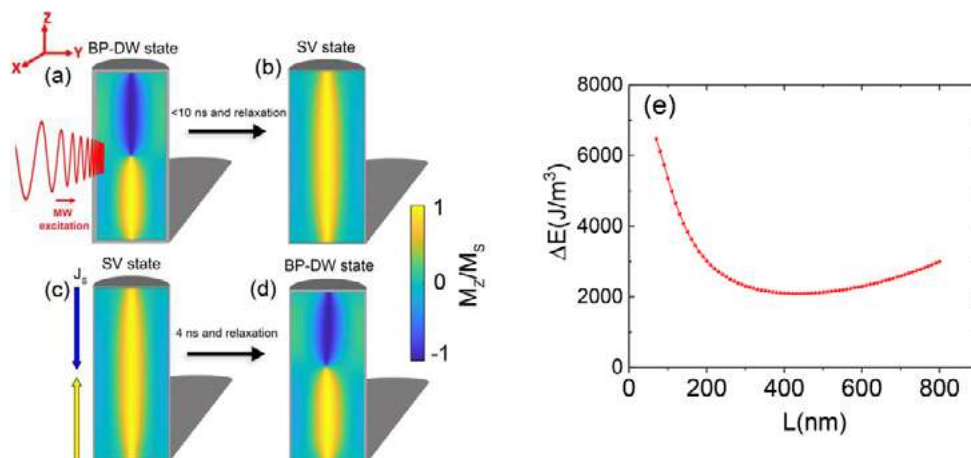


Figure 1: Cross section sequence of the m_z magnetization component of a 250 nm long NW, showing the used method to destroy the BP-DW state via a frequency-tuned mw field (a,b) and its posterior restoration using spin currents, (c,d). (e) Energy difference between the SV and BP-DW states against the length of the NW, proving a range of quasi-metastability between 200 and 400 nm.

Exchange bias alteration mediated by layers with perpendicular magnetic anisotropy

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The rise in the field of spintronics has augmented the efforts on developing more efficient devices for logic or memory applications. Some of these devices use Spin Valve (SV) [1] structures where exchange bias plays a crucial role. This well-known interaction is at the core of different devices and sensors such as hard drive reading heads, magnetic random access memories (MRAMs) or spin transfer torque MRAMs. The potential of this interaction together with the recent publication of Jenkins et al. [2] showing the atomistic origin of exchange bias and the experience in our group [3] have motivated us to study deeply this interaction under the influence of other interactions.

Here we show how granular exchange bias can be tuned depositing a Pt/Co/Pt stack with high Perpendicular Magnetic Anisotropy (PMA) on top of an IrMn layer of a top Spin Valve (SV). First-Order Reversal Curves (FORCs) are used here to study the coupling between these ferromagnetic stacks. Fig 1a show a FORC measurement of an SV where exchange bias is easily depicted. Moreover, Fig 1b shows a FORC measurement of the PMA stack deposited on top of the SV. Here we can identify the tuning of the exchange bias due to the influence of the PMA stack on the antiferromagnetic layer. This exchange bias alteration can be used as a pinning point of Domain Walls in spintronic devices.

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Figures

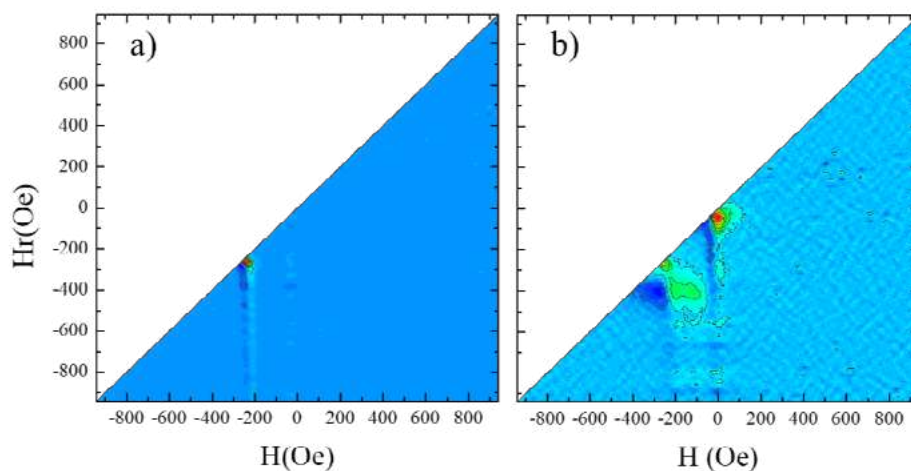


Figure 1: First Order Reversal Curve (FORC) diagram measured along the biased axis of a top Spin Valve with structure Ta(3)/NiFe(3)/CoFe(2.5)/Cu(2)/Ru(0.8)/CoFe(2.5)/IrMn(8)/NiFe(2.3)/Ru(3) (a). FORC diagram of the SV/PMA thin film showing an alteration in the exchange bias (b).

Spintronic devices based on domain wall logic

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The emerging field of magnetic logic seeks to redesign the principles of micro-electronics logic operations at the lowest level to use ferromagnetic materials directly. A submicrometer planar wire made from a soft ferromagnetic alloy has shown to be an excellent conduit for a domain wall; a domain wall can propagate in complex networks based on this type of wire under an external magnetic field that rotates in the plane of the device acting as a clock and a power supplies. A Permalloy($Ni_{88}Fe_{20}$) wire is investigated here: the domain wall dynamics in the wire are studied by a micromagnetic software “MUMAX3” to solve the Landau-Lifshitz-Gilbert.

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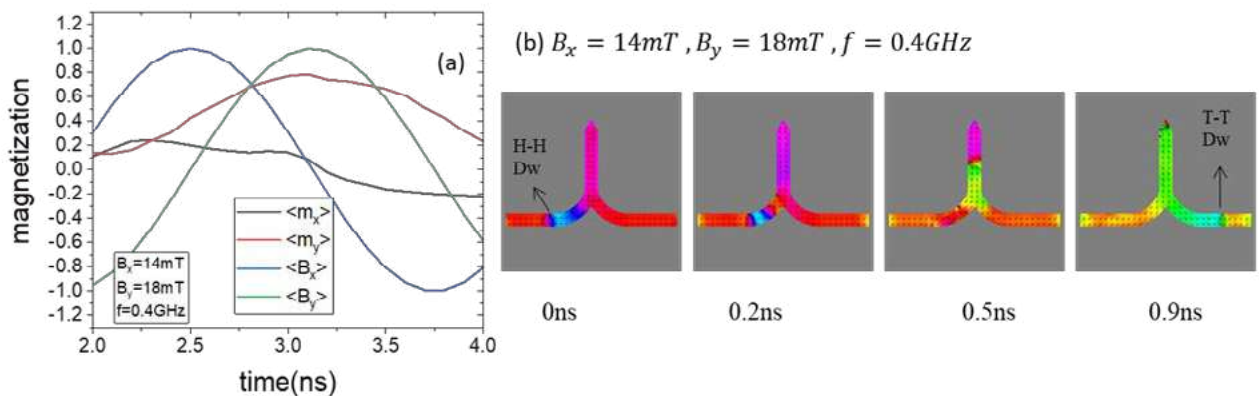


Fig1. Shows a NOT gat design.,(a) is the temporal evolution of the x-component and y-component of the averaged magnetization : ($\langle m_x \rangle$ vs .time and $\langle m_y \rangle$ vs .time) as well as the temporal evolution of the in-plane components of the elliptic rotating magnetic field ($B_x=14mT$ $B_y=18mT$) at a frequency of $f=0.4GHz$. (b) illustrates the micromagnetic snapshots (with MUMAX3) at the different instant of time showing the expected behavior of the DW moving in a NOT gate: starting with input as a head-to-head domain wall (H-H DW.) and driven along the sample by a rotating elliptic magnetic field resulting a tail-to-tail domain wall (T-T DW) as an output which is a perfect demonstration of a NOT logic operation.

Manipulation and characterization of cell spheroids by photovoltaic ferroelectric platforms

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Optoelectronic platforms, based on the bulk photovoltaic effect (PVE) presented by certain ferroelectrics have emerged as a versatile tool to manipulate and/or trap micro- and nano-objects [1]. Very recently, a method for manipulating aqueous solution droplets has been demonstrated with biological samples containing DNA and sperm [2]. In this work we report the action of these platforms on the manipulation of a different kind of relevant bio-species: multicellular spheroids. Spheroids are 3D cell models, with a diameter of hundreds of microns, whose cellular metabolism is closer to the one of tissues than monolayer cultures. Two cell lines of human cancer, MCF-7, from breast epithelial tissue (adenocarcinoma) and U-87mg from a brain epithelial tissue (glioblastoma astrocytoma), have been used to grow the spheroids.

In the experiments (see figure 1), droplets of cell culture medium containing a single spheroid are deposited in the air-paraffin interphase. When the light is switched on, a PV electric field is generated inside the substrate that extends outside it. This field has been able to manipulate the spheroid-droplet system, a hybrid bio-droplet quite different from the homogeneous droplets used in previous reports [2]. Attraction and trapping at the light position, or repulsion from it have been obtained depending on the different ferroelectric substrate face exposed to the light. An analysis of the droplet migration behaviour for the two cell lines and for a reference droplet with only cell culture medium has been carried out. The results show that the culture medium droplet is positively charged whereas the spheroids provide negative charge to the hybrid system.

This work has been funded by MCIN/AEI/10.13039/501100011033 under the grants PID2020-116192RB-I00, PID2019-110632RB-I00 and TED2021-129937B-I00

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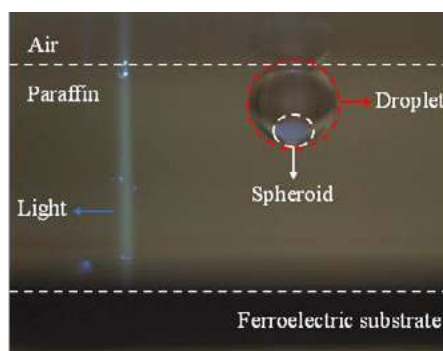


Figure 1: Schematics of the PV ferroelectric platform showing the hanging droplet containing the spheroid. The ferroelectric substrate is illuminated with a laser beam that generates a PV electric that manipulates the droplet.

Resistance Switching in Freestanding BaTiO₃ Layers

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Transition-metal oxides have received much attention due to their wide range of coupled responses emerging from strong electronic correlations [1]. Nonetheless, the restrictions imposed by epitaxial growth of these materials onto a limited number of single crystalline substrates has limited their functionalization and assembly with more application-relevant materials. The recent success in the fabrication of freestanding oxide layers has opened interesting opportunities of ampler material combinations and new device functionalities [2-3].

In our work, freestanding films of the ferroelectric oxide BaTiO₃ with widths down to 15 nm have been released from the substrate and functionalized in junctions with metal electrodes. Perpendicular electric transport measurements across these freestanding sheets have displayed a non-volatile resistive switching behaviour with memristor functionalities (one of the main requirements in neuromorphic circuits). The optimization of these memristive effects through the combination of these layered oxides with other materials families is expected to inspire novel device concepts contributing to improve the energy efficiency of big-data.

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(TaSe₄)₃I: Reconciling transport, optics and ARPES

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Recently, the quasi one-dimensional transition metal tetrachalcogenide (TaSe₄)₃I has been found to display the coexistence between superconductivity and ferromagnetism [1]. This result is conflicted with the previous works on this material, which overall predict it to be insulating [2]. Furthermore, no consensus exist on the electronic properties of (TaSe₄)₃ in the literature, since ARPES and transport measurements disagree by an order of magnitude on its electronic bandgap. In this work, we rationalize the observed transport gaps and reconcile them with ARPES and optical experiments by relating the dissimilarities with band-folding due to an approximated translational symmetry originated by a distortion caused by Se cages. Finally, we relate the observed superconducting behavior to a possible extrinsic hole doping which can tune the Fermi level through a Van Hove singularity.

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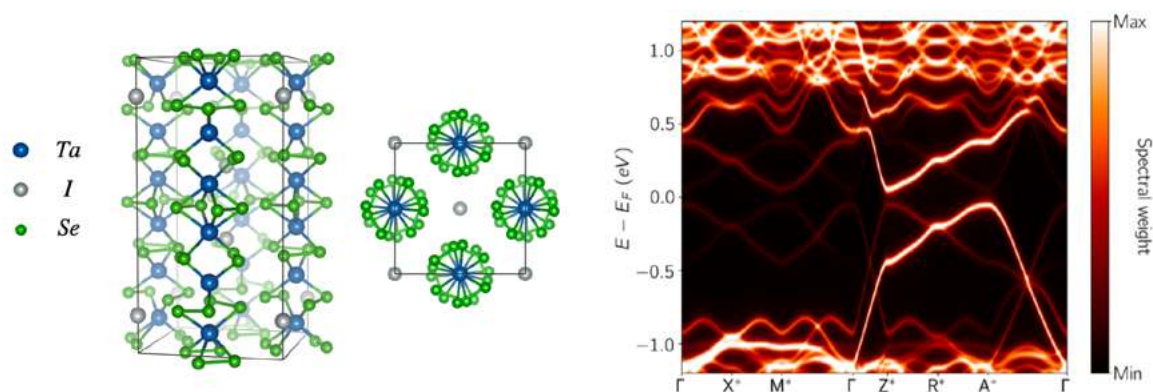


Figure 1: (TaSe₄)₃ structure (left) and unfolded bandstructure of the compound taking into account the distortion caused by Se cages (right).

Magnetization Reversal Processes of Highly Anisotropic Corrugated Thin Films

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Nano-undulated ferromagnetic (FM) thin films are of interest in fields such as magnonics or sensing due to their ease to tune magnetic anisotropy [1]. Traditionally, their magnetic behavior has been understood by means of Schlömann's dipolar field model for softly corrugated systems [2]. Moreover, FM corrugated thin films are able in certain conditions to sustain surface-plasmon polariton (SPP) excitations, forming magnetoplasmonic crystals [3,4].

We report on the magnetization reversal processes detected in permalloy films deposited onto highly corrugated patterns (250 nm in periodicity, 180 nm in amplitude) [Figure 1]. We observe an increasing switching field with FM layer thickness ($H_s \propto t$), opposed to Schlömann's prediction of $H_s \propto 1/t$. We reproduce our experiments qualitatively with micromagnetic simulations, finding that the magnetic behavior has a dipolar origin and does not follow Schlömann's predictions even at FM thicknesses larger than the ripple amplitude. These results demonstrate that the traditional dipolar based approaches are incomplete in highly corrugated thick samples and will help to get a better understanding of operating mechanisms in magnetic field sensors based on undulated ferromagnetic materials. Additional reflectance characterization of these materials is currently in progress in order to determine magnetoplasmonic effects in these materials.

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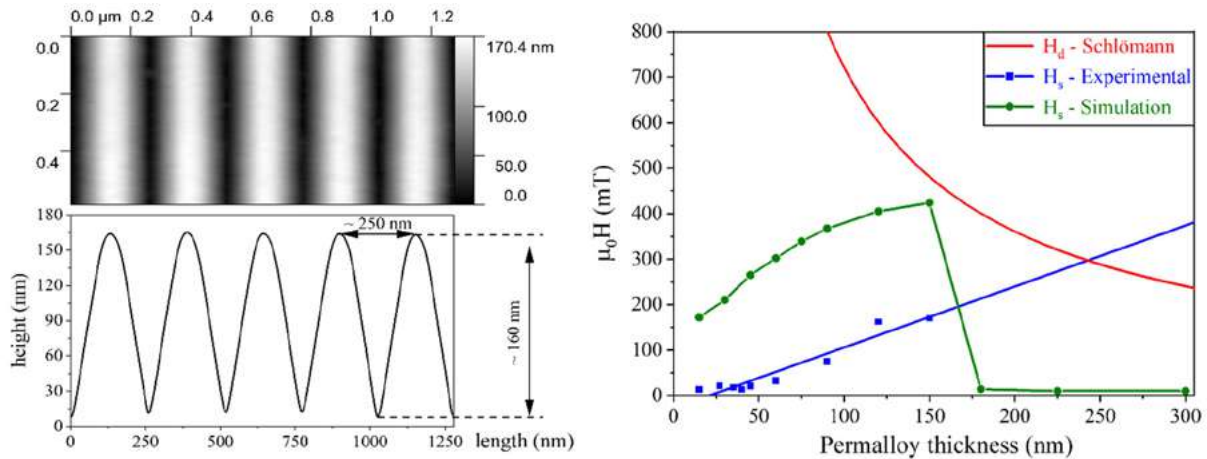


Figure 1: Left: AFM image and profile of sawtooth patterned Si substrate. Right: Experimental (blue) and simulated (green) switching field H_s evolution with FM layer thickness t . Schlömann's dipolar field estimation (red) is shown as reference.

NdNiO₃-BaTiO₃ Ferroelectric Tunnel Junctions

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Oxide-based Ferroelectric Tunnel Junctions (FTJs) are interesting devices for neuromorphic computing since they exhibit ferroionic memristive behavior [1,2,3]. We investigate a new degree of freedom for this kind of devices linked to the sharp metal to insulator transition (MIT) displayed by rare earth nickelates. Exploring the role of the strong electronic correlations and the MIT on the perpendicular transport of FTJs would be not only intriguing from a fundamental point of view but could yield interesting new concepts for devices [1,4].

We are able to grow high quality –epitaxial and flat– NdNiO₃ thin films with different degrees of epitaxial strains, what allows us to tune the critical temperature of the NdNiO₃ MIT in a wide range. In the present work, we have fabricated FTJs with BaTiO₃ as the nanometric ferroelectric tunnel barrier, NdNiO₃ as bottom electrode and Au as top electrode.

NdNiO₃-BaTiO₃ based FTJs show a tunnel electroresistance (TER) of $TER = 10^5$ %. Our FTJs exhibit memristive behaviour, featuring multilevel resistance states which can be reached and stabilized with simple voltage sequences. We have explored the role and possible interplay between the different ferroelectric and ferroionic effects to tailor synaptic responses as required in neuromorphic computing [2].

Future work will be devoted to progress in the emulation of synapses and neurons functionalities using these devices.

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Tunable ferromagnetic order in 2D layered transition metal dichlorides

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Metal dihalides MX_2 , where M is a transition metal and X a halogen, are a class of 2D layered materials bonded through van der Waals interactions. These binary compounds exhibit magnetic texture with semiconducting electronic properties. Since single layers can grow epitaxially on metal substrates, there is a strong interest in determining whether these properties persist at the 2D limit [1].

Here we study the epitaxial growth of FeCl_2 and NiCl_2 on an Au (111) substrate. Their chemical and electronic properties were explored by low-energy electron diffraction, X-ray photoelectron spectroscopy and low-temperature scanning tunneling microscopy and spectroscopy. These 2D materials are arranged in large and flat monolayers, which apparently are highly decoupled from the substrate. The magnetic properties of the dihalides were studied by X-ray absorption spectroscopy, revealing a ferromagnetic order related to the 3d electrons of the transition metals, which survives on a metallic substrate. Interestingly, the magnetic alignment depends on the transition metal used, so that it can be switch from perpendicular to in-plane by substituting the metal ion from iron to nickel. In addition to this, their thermal stability and large electric gap make them suitable candidates in many applications, such as thin heterostructures in magnetoelectric devices or as a barrier to decouple molecular systems from the conductive substrate and experimentally access to new magnetic properties in the low dimensional limit.

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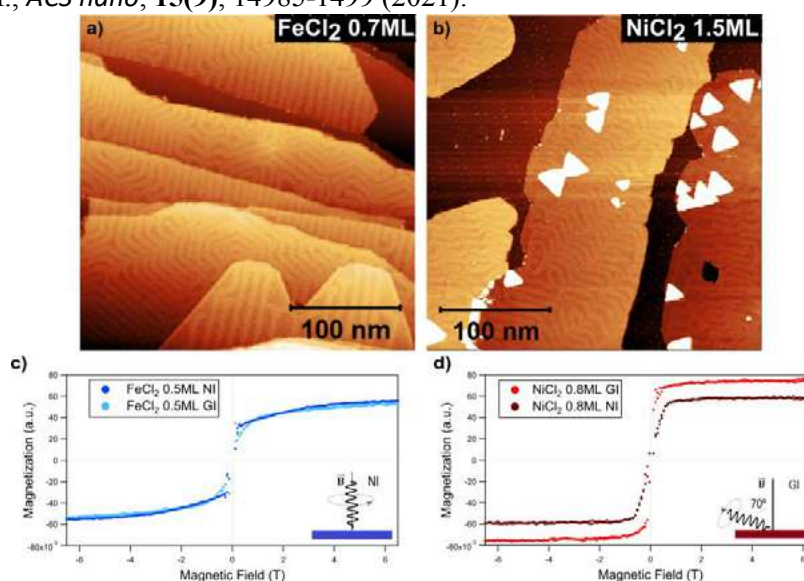


Figure 1: STM and AFM images on FeCl_2 (a) $I=20\text{pA}$ $U=3.0\text{V}$) and NiCl_2 (b) $I=10\text{pA}$ $U=2.0\text{V}$). Comparison of magnetization loops for FeCl_2 and NiCl_2 at normal incidence 0° (NI) and grazing incidence 70° (GI) measured at the Fe L_3 edge (c) and Ni L_3 edge (d). The inset represents a scheme of the incidence angle of the easy axis of magnetization direction respectively.

Study of Spin-to-charge conversion effect in ferromagnet/2DEG based nanodevices: The reading section of the MESO device

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The Magnetoelectric Spin-Orbit (MESO) technology [1] is a relatively new technology coming from the Spin Orbitronics field. MESO devices combine the advantages of the Magnetoelectric effect (ME) (input of the device) and Spin Orbit coupling (SOC) (read out part), to achieve an efficient Spin-to-charge conversion (SCC) and the capability of storing non-volatile information in the magnetic state of the device. In this work, we focus on the MESO device's read-out part, using a 2-dimensional electron gas (2DEG) as a high SOC material [2]. The two principal advantages of using 2DEGs are the finite Rashba SOC they present, and the high tunability of their electronic structure, which is related to the Rashba-Edelstein effect (IREE) response [3]. This section consists of applying a charge current through a ferromagnetic material, which is equivalent to the generation of the spin current via the ME, and this current will flow from the ferromagnet into the high SOC material. Due to the presence of inverse IREE, which naturally appears in 2DEGs [4,5], the spin polarized current will be transformed into a perpendicular charge current that will carry the information about the magnetization of the ferromagnet. In our study, we have designed, patterned and fabricated T-shaped nanodevices where the charge current is injected into a Co layer (the ferromagnet), and there it is transformed into a spin polarized current that will flow into the 2DEG, generating a perpendicular voltage output. Interestingly, we found signatures of SCC and studied its evolution as a function of the temperature while applying back-gate, external magnetic-field or while rotating the sample. Furthermore, since the current injected into the 2DEG is not a pure spin current, but a mixture of spin and charge currents (i.e. a spin-polarized current), we tried to disentangle the IREE contribution from different spurious effects like Planar Hall Effect, Anomalous Hall Effect and anisotropic magnetoresistance. Our findings are very promising in terms of spin-logic approaches for alternative applications in computing field, paving the way towards a new generation of scalable, non-volatile and high energy efficiency beyond-CMOS spintronic logic devices.

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Dragging of Berry curvature in ferromagnetic Weyl semimetals NiMnSb and PtMnSb

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The Anomalous Hall effect (AHE) is an intriguing transport phenomenon in ferromagnets, which exhibit longitudinal currents even in the absence of a magnetic field, as opposed to the ordinary Hall effect [1]. The AHE was first understood as an intrinsic effect by Karplus and Luttinger [2], showing that the inner magnetization of ferromagnets breaks Time Reversal Symmetry, allowing the antisymmetric part of the linear response tensor to be finite, as required by Onsager's relations. This quantity is proportional to what we nowadays know as Berry curvature. Therefore, the non-trivial topology of the band structures is the responsible of the intrinsic AHE [1]. As a result, topological features, such as nodal lines or points, close to the Fermi energy have a deep impact in the transport properties of these materials, leading to huge Anomalous Hall Conductivities (AHC). This has been a well-established paradigm for the last years for the linear AHC.

In the present work, we study the AHC in the half-Heusler ferromagnets NiMnSb and PtMnSb. We conclude that the big AHC present in these Heusler compounds is indeed due to the presence of topological features (Weyl nodes), but which appear away from the Fermi level. By combining the *ab initio* calculations with a toy-model, we show that the steep slope-bands both compounds exhibit are capable of dragging the BC originated in the Weyl nodes down to the Fermi level, leading to the huge AHC. We propose that this dragging effect of the Berry Curvature can be generalized to other materials exhibiting this band structure behavior, enriching the paradigm described above. Further research in this direction is currently being done.

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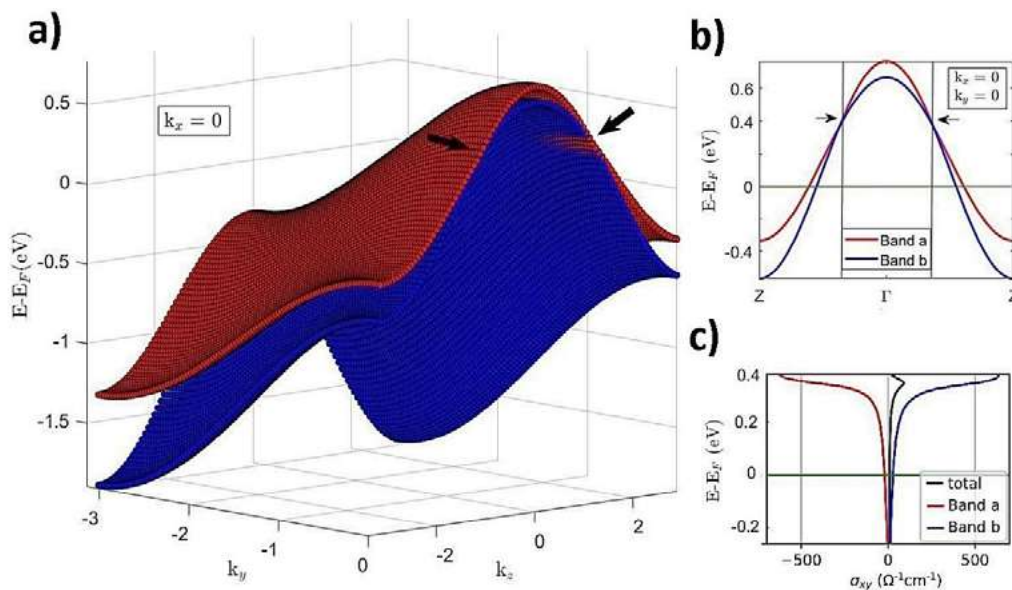


Figure 1: *Ab-initio* calculations reveals NiMnSb and PtMnSb to be Weyl semimetals with Weyl nodes near and far from Fermi level. To observe the effect of non-trivial topologies, one should expect nodes near to Fermi level. However, in these systems, band dispersions are steep resulting in dragging of Berry curvature to the Fermi level even though Weyl nodes are far from Fermi level. This can be seen with the present toy-model, in which the Weyl nodes (black arrows in a) and b)) lead to a finite AHC at the Fermi level (c)).

Direct magnetic evidence, functionalization and low-temperature magneto-electron transport in liquid-phase exfoliated FePS₃

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Magnetism and the existence of magnetic order in a material is determined by its dimensionality. In this regard, the recent emergence of magnetic layered van der Waals (vdW) materials provides a unique playground to explore the exotic magnetism arising in the two-dimensional (2D) limit. The magnetism of 2D flakes has been commonly studied by indirect methods like Raman spectroscopy. Here, taking advantage of liquid-phase exfoliation (LPE) method, we show a first direct magnetic evidence of the antiferromagnetic transition in FePS₃ few-layer flakes, performed with a SQUID magnetometer (Figure 1a). It is concomitant with a clear reduction of the Néel temperatures with the flake thickness, in contrast with previous Raman reports.[1]

The quality of the LPE FePS₃ flakes allows the study of electron transport down to cryogenic temperatures (Figure 1b,c).[2] The significant through-flake conductance is sensitive to the antiferromagnetic order transition. Besides, an additional rich spectra of electron transport excitations, including secondary magnetic transitions and potentially magnon-phonon hybrid states,[3] appears at low temperatures (Figure 1d). Finally, we show that the LPE is additionally a good starting point for the mass covalent functionalization of 2D magnetic materials with functional molecules.[4] This technique is extensible to any vdW magnetic family.

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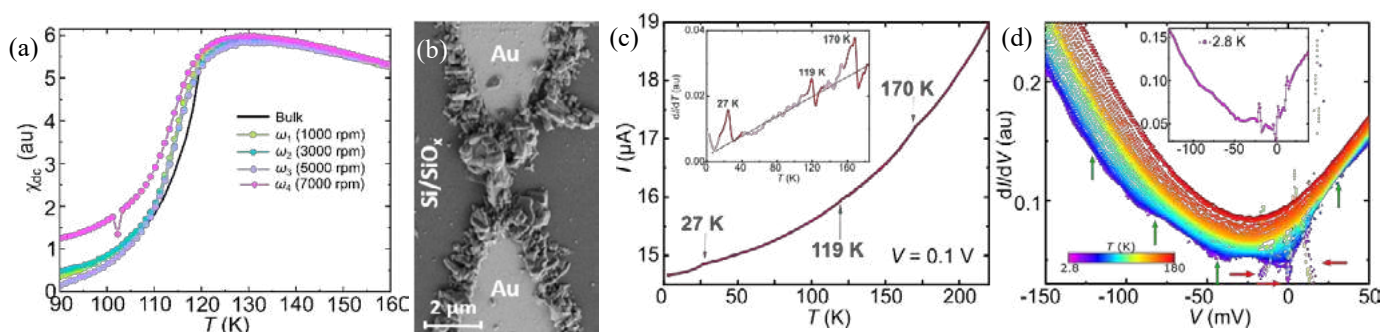


Figure 1: (a) First derivative of magnetic susceptibility (χ) measured as a function of temperature in a bulk reference sample and exfoliated samples ω_1 , ω_2 , ω_3 and ω_4 . (b) Scanning Electron Microscopy (SEM) image of a representative electrode pair containing LPE FePS₃ flakes (ω_1) trapped by dielectrophoresis (DEP). (c) Current I – Temperature T characteristics measured on a FePS₃ device at a fixed $V = 0.1$ V and its first derivative (dI/dT) (inset). (d) First derivative (dI/dV) of the Current I – Voltage V characteristics at different temperatures.

Size-dependent dipolar ferromagnetism in micro- and nano-molecular crystals

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We study experimentally how crystal size influences magnetic ordering in arrays of molecular nanomagnets coupled by dipolar interactions (Fig. 1, left). Compressed fluids techniques [1] have been applied to synthesize crystals of Mn_6 molecules (spin $S = 12$) with typical sizes ranging from 28 μm down to 220 nm (Fig. 1, centre). The onset of ferromagnetic order and the spin thermalization rates have been studied by means of micro-SQUID ac susceptibility measurements. We find (Fig. 1, right) that the ordered phase remains ferromagnetic, as in bulk [2], but the critical temperature T_c decreases with crystal size. Simple magnetostatic energy calculations, supported by Monte Carlo simulations, account for the drop in T_c in terms of the minimum attainable energy for finite-size magnetic domains limited by the crystal boundaries. Frequency-dependent susceptibility measurements give access to the spin dynamics. Although magnetic relaxation remains dominated by individual spin flips, the magnetic order leads to very long spin thermalization time scales. The results show that size influences the magnetism of dipolar systems [3] with as many as 10^{11} spins and are relevant for the interpretation of quantum simulations performed on finite lattices.

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Figures

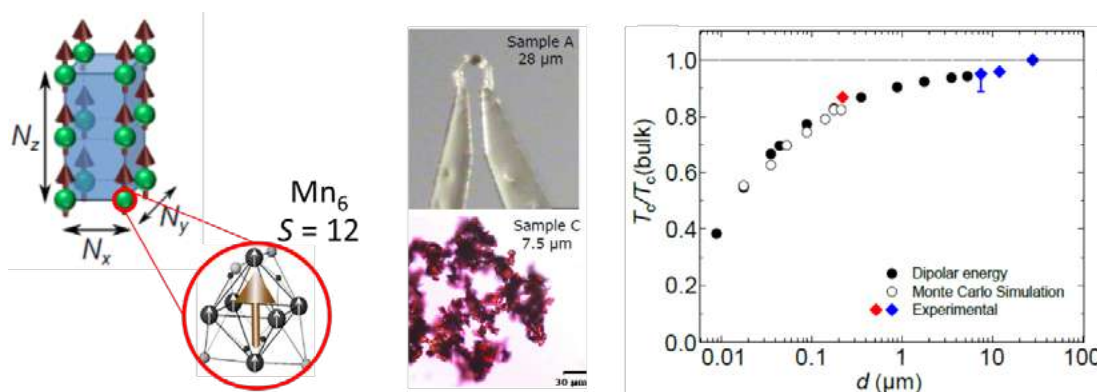


Figure 1. Left: Schematic view of a lattice of Mn_6 molecular nanomagnets, each with a spin $S = 12$, interacting via dipolar interactions [2]. **Centre:** Microscopy images of two samples of size controlled Mn_6 crystals. **Right:** Dependence of the ferromagnetic ordering temperature, normalized to the bulk or thermodynamic value, as a function of crystal size.

Automatic procedure to obtain tight-binding parameters for second-principles simulations. The case of SrTiO_3

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First-principles calculations allow to compute the energy and properties of a compound from essential information about its structure and composition. In principle, even the finite temperature behavior of materials is accessible from first-principles simulations since the early stage of density functional theory (DFT). Nowadays, however, such simulations remain practically limited by computational resources to very small length scales (a few hundreds of atoms per cell) and timescales (a few picoseconds). Nevertheless, many important fundamental and applied problems require to explore these large time and length scales at operating conditions (finite temperature, electric fields, etc). A practical way to overcome these limitations is to work with effective atomistic models, integrating out the electronic degrees of freedom and providing a simple parametric description of the Born–Oppenheimer energy surface in terms of structural degrees of freedom. This might be a constriction in some cases, specially, in those problems where the relevant physics is dominated by the electronic degrees of freedom. Recently, a method has also been proposed to reintroduce explicitly the treatment of the meaningful electronic degrees of freedom in the form of a tight-binding model, while avoiding double-counting with the effective atomic potentials [1].

This tight binding approach is based on the Taylor expansion of the DFT energy around a reference electronic density. The deformation density with respect this reference, as well as the hamiltonian matrix elements, is expressed in a basis of Wannier functions which are obtained from the band manifolds of interest in the problem. Only the relevant electrons to the problem can be retained in the description, reducing by orders of magnitude the computational cost. This gain in efficiency would come at the cost of finding the right parameters in the tight binding hamiltonian matrix elements, that would reproduce as close as possible the first-principle hamiltonian matrix elements.

Here we propose a method implemented in python, the MODELMAKER code, for the automatic parametrization of such tight binding hamiltonian. The starting point is made of first-principles calculations (from the SIESTA code [2]) in training sets with a small number of atoms in the unit cell. Since there is not input coming from the experiment, our method retains full predictive power, and that is why it is coined as second-principles simulations. Both electron-lattice coupling, studied by calculations characterized by geometry distortions, and electron-electron interactions, caught by simulations exploring electronic states beyond the Born–Oppenheimer surface, are included in the parametrization of the electronic model. The obtained parameters are validated comparing the band structures computed from first and second-principles in configurations that are not included in the training set. This methodology has been applied to a paradigmatic functional oxide such as SrTiO_3 .

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Optimizing the performance of IrO₂ thin films by doping with Co

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Iridium Oxides have been proven to be very useful in spintronics. Indeed, a decade ago, IrO₂ was proposed as the most promising material for spin-current detectors; thanks to its strong spin-orbit coupling and concomitant large spin Hall effect.[1] Doping this material with magnetic elements opens the possibility of tuning its electrical and magnetic behavior and/or the efficiency of the conversion between charge currents and spin currents, of interest for several spintronic applications.

In this work we have explored the role of Co doping on the structural and magnetic properties of IrO₂ thin films. Ir_{1-x}Co_xO₂ (x = 0.07–0.6) 80 nm thin films were prepared by reactive magnetron co-sputtering and analyzed using X ray reflectivity and diffraction, Scanning Electron Microscopy and SQUID magnetometry.

We've found that, regardless of the doping, the rutile-like crystal structure of IrO₂ was maintained; with only gradual cell contraction and grain size reduction as doping increases. On the other hand, and despite the high Co doping achieved, no ferromagnetism was observed in any of the samples. From this, one can infer that cobalt takes a Co³⁺ oxidation state in a low spin configuration, inducing a change of oxidation state of the iridium ions from Ir⁴⁺ to Ir⁵⁺. This is expected to result in a higher spin-orbit coupling and, therefore, making Ir_{1-x}Co_xO₂ thin films promising candidates for devices with optimum conversion between charge currents and spin currents [2].

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Thermal transport on few-layers Fe₃GeTe₂

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Understanding thermal transport in van der Waals (vdW) materials is required for future applications of these novel materials. However, despite recent efforts, the physics of thermal transport on a few layers of vdW materials is not well comprehended, mainly how heat transport is affected by material thickness, substrate, interfaces, and phase transitions. In this work, we present out-of-plane thermal conductivity (κ) and thermal boundary conductivity (TBC) of a few layers of Fe₃GeTe₂, which recently have attracted great research interest due to experimental findings of rare two-dimensional ferromagnetism close to room temperature[1]. Measuring the dependence of κ on the thickness and temperature, we discuss the ballistic and diffusive phonon transport for Fe₃GeTe₂ and vdW materials in general, also discuss the mechanism of the sudden change of κ observed at Curie temperature (~ 200 K) which is robust to external magnetic fields up to 50mT, which is the field able to switch between stripe domains and uniform magnetized states[1].

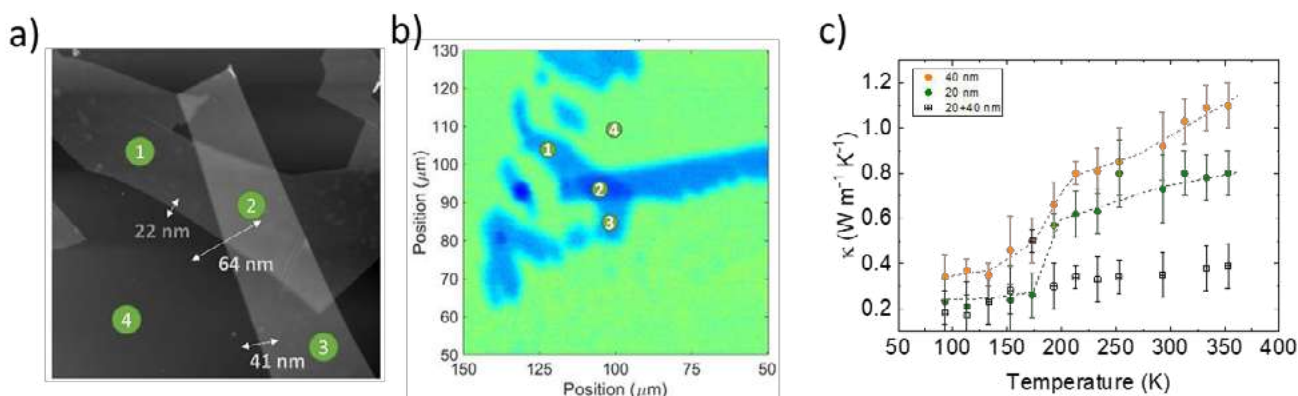


Figure 1: a) Atomic Force Microscopy of Fe₃GeTe₂ flakes with different thicknesses. b) Phase contrast on Frequency-Domain thermoreflectance (FDTR) due to the thickness and κ variations c) κ vs Temperature in the points 1, 2, and 3 of a) and b).

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Tailoring the magnetization processes of chemically modulated cylindrical nanowires

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The control of the magnetization processes along elongated structures is key for the development of novel magnetic devices. Recent studies shown that complex and interesting spin textures and novel physics phenomena can be observed in cylindrical nanowires [1]. Electrodeposition is a versatile tool for the synthesis of cylindrical nanowires with controlled morphology and composition [2]. We will show how local changes in composition along the axial direction in permalloy nanowires act as pinning sites for controlling the domain wall motion [3] producing also complex tridimensional spin textures with well-defined chirality [4].

Compositional gradients can be also introduced by gradually changing the Fe/Ni ratio, producing an asymmetrical landscape for domain wall motion, which is reflected in asymmetrical magnetization processes under applied magnetic field. Figure 1 shown a comparison of First Order Reversal Curves (FORC) measured in homogeneous and modulated nanowires, with a clear asymmetry in the curve in the latter ones. Moreover, we are able to introduce another degree of freedom by modulating the composition along the radial direction (FeNi/Au/Co nanowires) in which the coupling between magnetic layers and thus the magnetic properties are controlled by the thickness of the Au layer.

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Figures

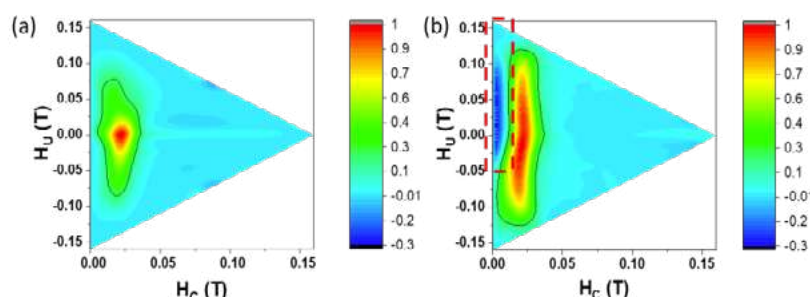


Figure 1: FORC diagrams measured a) in permalloy nanowires and (b) in nanowires in which an axial gradient of composition has been introduced. The asymmetry of the magnetization process is clearly shown in the area marked with the red square.

Hybrid optical-electrical sensing of memristors based in LSMO/BTO/ITO ferroionic tunnel junctions

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The sensing of the non-volatile resistive states of large arrays of memristors is an important challenge for the implementation of energy efficient neuromorphic computing. The reversible build-up of a Schottky barrier is the dominant mechanism of the resistive switching in one kind of FerroIonic Tunnel Junctions, originating the different memristive states [1]. In this work we take advantage of the Schottky barrier to get an active reading of the memristive states in a $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{BaTiO}_3/\text{ITO}$ ferroionic tunnel junction with a 3 nm thick BaTiO_3 layer [2,3]. The Schottky barrier formed in the BaTiO_3 layer dramatically enhances its optical response and produces a photovoltaic response when illuminated with a UV LED. The open circuit voltage V_{oc} correlates linearly with the resistance of each state, facilitating the active sensing of the memristive state and opening the way to an ultra-low energy sensing of the devices enabling a parallel implementation.

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Figures

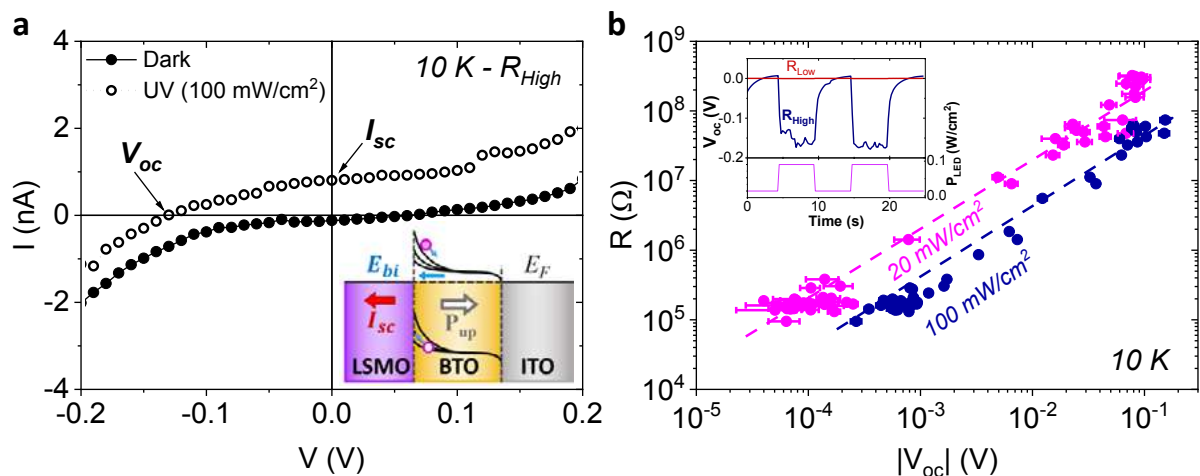


Figure 1: (a) I-V curves in the R_{High} in dark and under UV illumination. Inset is a sketch of the band diagram, indicating the variation of the Schottky barrier for different memristive states. (b) Resistance of different memristive states at 10 K as a function of the measured $|V_{oc}|$, for two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

Magnon currents excited by the spin Seebeck effect in ferromagnetic EuS thin films

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Magnons, the collective bosonic excitations in magnetically ordered systems, allow for the transport of spin angular momentum even in insulators. The ability to control the generation, propagation, and detection of such magnon spin currents represents an asset for the progress of spintronics. So far, magnon transport has been studied mainly through $\text{Y}_3\text{Fe}_5\text{O}_{12}$ (YIG) and a few other ferri- and antiferromagnetic insulators [1], while there exist many materials in which their behaviour is little known. Here, we study for the first time the generation of thermal magnon currents in ferromagnetic insulator europium sulphide (EuS), which exhibits a Curie temperature $T_c = 19$ K in thin films [2]. We perform both local (LOC) and non-local (NL) transport measurements in 18-nm-thick films of EuS using Pt electrodes, with different separation distances d , as magnon injectors and detectors. We study the voltage response generated at the detector due to the inverse spin Hall effect, given that spin angular momentum is transferred through the Pt/EuS interface. We identify the magnon induced spin currents by measuring the dependence of the second harmonic component of this voltage on the in-plane angle (α) applying an external magnetic field $\mathbf{B}$ that orients the EuS magnetization $\mathbf{M}$ and determines the spin current spin polarization. The observed LOC and NL signals indicate that magnon currents can be excited thermally by the spin Seebeck effect. By comparing the dependence of the LOC and NL signals with the temperature ($2 \text{ K} < T < 30 \text{ K}$) and magnetic field ($< 9 \text{ T}$), we confirm the magnon transport origin of the NL signal. By studying the NL signal as a function of d , we extract the magnon diffusion length in the EuS films ($\sim 140 \text{ nm}$), which we find to be much shorter than the YIG case. We discuss our results considering the Gilbert damping and the T_c of the EuS films.

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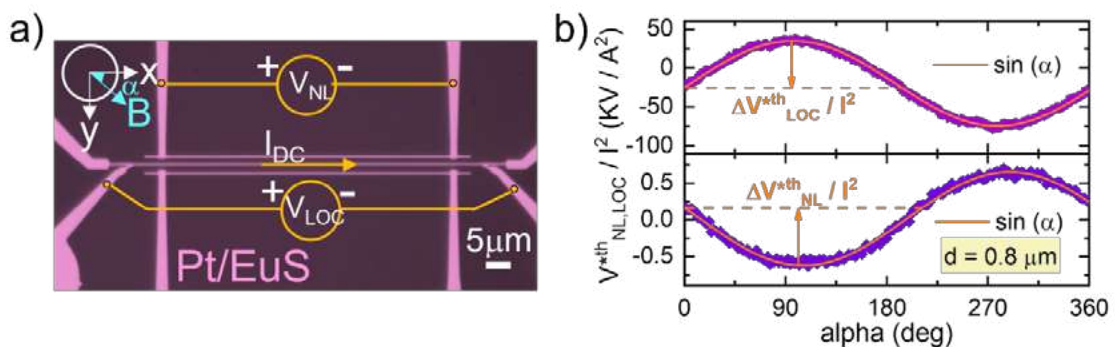


Figure 1: a) Optical microscope image of a device showing the measurement configuration. b) Representative LOC and NL angular dependent signal detected for thermally excited magnons at 2 K and 0.3 T.

Spin-to-charge conversion in $\text{Bi}_x\text{Se}_{1-x}$ from all-electrical nanostructured devices

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Materials with a strong spin-orbit coupling present some effects relevant for the development of spintronics devices, such as the spin Hall effect (SHE) and its inverse (ISHE) which result in conversion between charge currents and spin currents. The efficiency of spin-to-charge current conversion is given by the spin Hall angle θ_{SH} [1]. Large θ_{SH} has been reported in sputtered amorphous $\text{Bi}_x\text{Se}_{1-x}$ [2]. Amorphous $\text{Bi}_x\text{Se}_{1-x}$ is thus a promising material that can be used in the recently proposed magneto-electric spin-orbit (MESO) logic device by Intel [3], in which not only large θ_{SH} is needed, but also a high resistivity [4]. One approach using electrical spin injection in nanostructured devices have been reported using local configuration [5]. However, we need to properly estimate the spin diffusion length (λ_{SD}) for a more accurate quantification of θ_{SH} . By using a non-local configuration with lateral spin valves (LSV), we can perform two distinct measurements and independently extract θ_{SH} and λ_{SD} . We were able to fabricate sputtered amorphous $\text{Bi}_x\text{Se}_{1-x}$ nanostructures and integrate them in LSV devices by multiple e-beam lithography steps. This is a challenging process that requires a comprehensive understanding of the interface between $\text{Bi}_x\text{Se}_{1-x}$ and the metals used in the LSVs, which is an extremely critical factor to design an all-electrical spintronic device. By using the configuration shown in Fig. 1a, we successfully measure the spin Hall signal ($2\Delta R_{\text{SHE}}$), which allows us to quantify θ_{SH} in sputtered $\text{Bi}_x\text{Se}_{1-x}$ (Fig. 1b). In the same device, we also measured the spin signals using non-local configuration for the reference device and across the $\text{Bi}_x\text{Se}_{1-x}$ wire (Fig. 1c), that allow us to extract λ_{SD} .

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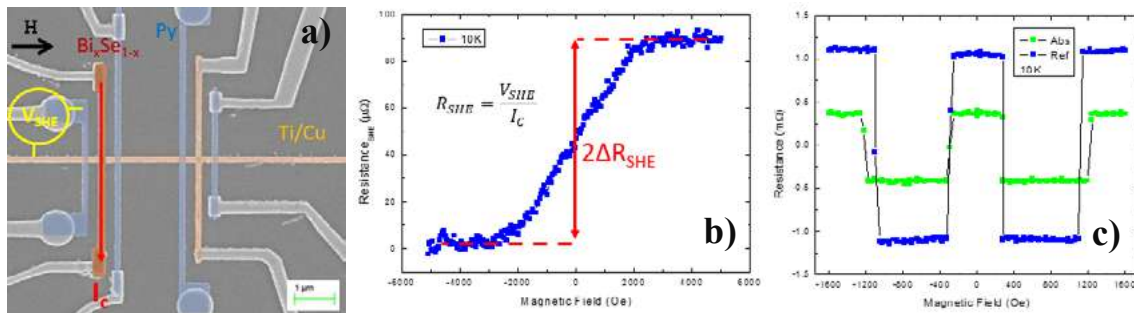


Figure 1: a) SEM image of two Py/Cu-based lateral spin valves: on the left with a middle wire for spin absorption of $\text{Bi}_x\text{Se}_{1-x}$ (30 nm) and on the right as a reference. b) SHE resistance as a function of the external magnetic field measured at 10 K using the configuration in panel a, demonstrating spin-to-charge conversion in a $\text{Bi}_x\text{Se}_{1-x}$ nanostructure. c) Non-local resistance as a function of the external magnetic field for the reference devices and across the $\text{Bi}_x\text{Se}_{1-x}$ wire at 10K.

Looking for the spin swapping effect

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As the electronics industry is reaching the fundamental limits of Moore's law with characteristic sizes of 7 nm in CMOS technology, new beyond-CMOS technologies are required to overcome the end of this law. One promising proposal to achieve this is spintronics, a field of electronics in which the intrinsic spin of the electron is exploited in addition to the fundamental electronic charge. Nowadays, one of the most used ways to create spins is by charge-to-spin current conversion effects, for example the spin Hall effect (SHE) [1], in systems with strong spin-orbit coupling (SOC). Reciprocally, spins can be detected by spin-to-charge current conversion from the corresponding inverse effects. Moreover, SOC gives rise to other interesting effects as the recently predicted spin current swapping (SCS) [2], a spin-to-spin conversion effect.

This work presents a study on the SCS effect, which has been theoretically predicted but so far not experimentally measured. For this purpose, a nanodevice based on a lateral spin valve (LSV) [3] has been designed, fabricated and characterized, which will allow the measurement of the SCS effect. The fabrication includes two electron-beam lithography (eBL) steps: the first one for patterning the ferromagnetic (NiFe) nanostructures, which will act as the spin injector and detector of the LSV, and the second one for the Cu channel, which will allow the spin transport. After measuring the reference spin signals, SOC-impurities, in this case Ga atoms, have been implanted in the nanodevice by focused-ion beam (FIB) which should give rise to the SCS effect [2]. The experiment reveals that the measured spin signal after the FIB treatment has a shift around zero magnetic field when compared to the reference signal, which is the expected outcome if the SCS effect would be present. This experimental observation is thus compatible with the presence of the SCS effect in our nanodevices based on Ga-doped Cu.

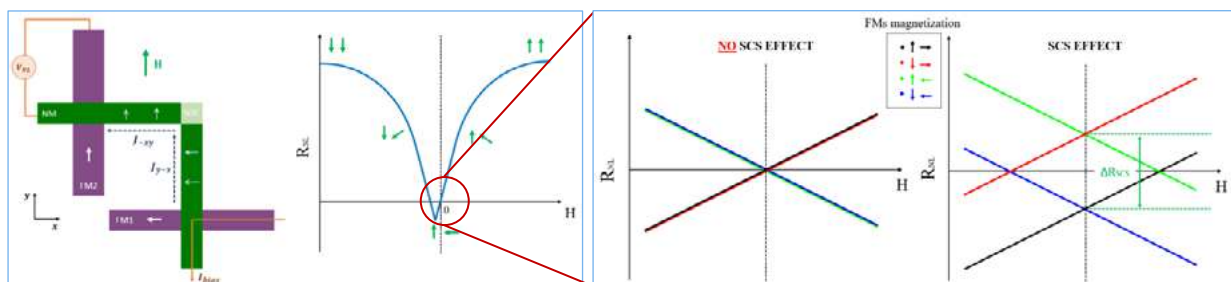


Figure 1: Left figure shows the designed nanodevice, the measurement configuration and the expected non-local spin signal. Right figure shows a more accurate measurement around zero magnetic field for the case where SCS is present and the case where it is not present, for the four possible magnetization configurations of the ferromagnets (FM).

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Modulating the magnetic properties of layered hybrid organic-inorganic metal-halide perovskites by chemical design

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Magnetic layered (2D) materials have awakened the attention of researchers since the isolation of intrinsically magnetic monolayers, and as result, the library of magnetic 2D materials is growing every day. Furthermore, one of the main goals in this field is to achieve control over their magnetic properties for their integration in devices^[1]. In this regard, layered hybrid organic-inorganic metal halide perovskites (HOIPs) present an ideal platform for magnetic tunability due to their chemical and structural versatility^[2-3]. Here we conducted a detailed study to understand the effect of the transition metal (Cu^{2+} , Mn^{2+} and Co^{2+}), organic spacer (alkyl- and aryl-ammonium) and perovskite phase (Ruddlesden-Popper and Dion-Jacobson) on their magnetic properties. We found that for Cu^{2+} HOIPs, an increase of in-plane anisotropy and a reduction of the interlayer distance lead to a change in their magnetic behavior from a 2D ferromagnet to a quasi-3D antiferromagnet (Figure 1). In contrast, the magnetism of Mn^{2+} HOIPs is intrinsically characterized by antiferromagnetic intralayer interactions. Finally, Co^{2+} crystals with a non-perovskite structure present a dominant paramagnetic behavior. Therefore, our results demonstrate that the chemical flexibility of HOIPs can be exploited to develop novel layered magnetic materials with tailored magnetic properties.^[4]

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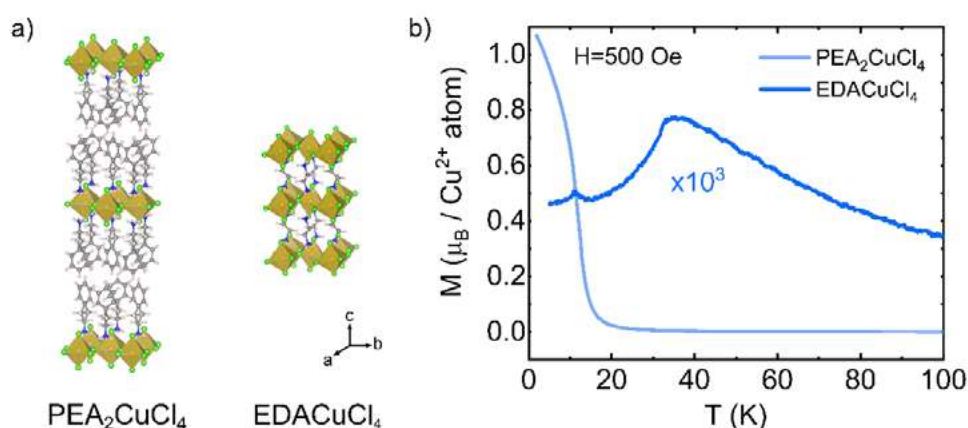


Figure 1: a) Crystal structures of PEA₂CuCl₄ (phenethylammonium – PEA) (CCDC 751958) and EDACuCl₄ (ethylenediammonium - EDA) (CCDC 1148696) drawn using VESTA software and b) their magnetization (M) versus temperature (T) with the field parallel to the $[\text{CuCl}_6]^{4-}$ octahedra layers.

Tuning the magnetism of NiPS₃ and MnPS₃ through organic ion intercalation

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Intercalation of van der Waals layered materials is a powerful processing tool to tailor their properties [1–3]. In these studies, we focused our attention on the modulation of the magnetic properties of two antiferromagnetic transition metal phosphorous trisulfides, NiPS₃ ($T_N = 155$ K) and MnPS₃ ($T_N = 78$ K), through electrochemical and/or exchange-based organic cation intercalation. In particular, NiPS₃ was successfully electrochemically intercalated with tetrabutylammonium ions (TBA⁺) and with cobaltocenium (Co(Cp)₂⁺) via spontaneous TBA⁺/Co(Cp)₂⁺ exchange in solution (Figure 1a)[4]. On the other hand, MnPS₃ was processed directly in aqueous solutions of four alkylammonium bromide salts (R₄N, with R₄ = tetramethyl, tetraethyl, tetrabutyl, cetyltrimethyl), leading to the corresponding hybrid organic-inorganic intercalates. X-ray diffraction, Raman, and gravimetric studies were carried out for structural characterizations. Finally, magnetic measurements revealed the suppression of pristine antiferromagnetism and the emergence of molecular-dependent ferrimagnetism for both the intercalated host materials, characterized by a hysteretic behavior with finite coercive field and remanent magnetization. We found that TBA_{0.25}NiPS₃ ($T_C = 78$ K) and [Co(Cp)₂]_{0.25}NiPS₃ ($T_C = 98$ K) show doping-induced magnetizations in the order of 10⁻² μ_B/atom (Figure 1b) [4]; meanwhile, the four R₄N-MnPS₃ intercalates ($T_C \sim 45$ K) display a guest's size-dependent magnetism with saturation magnetization reaching up to 1 μ_B/atom.

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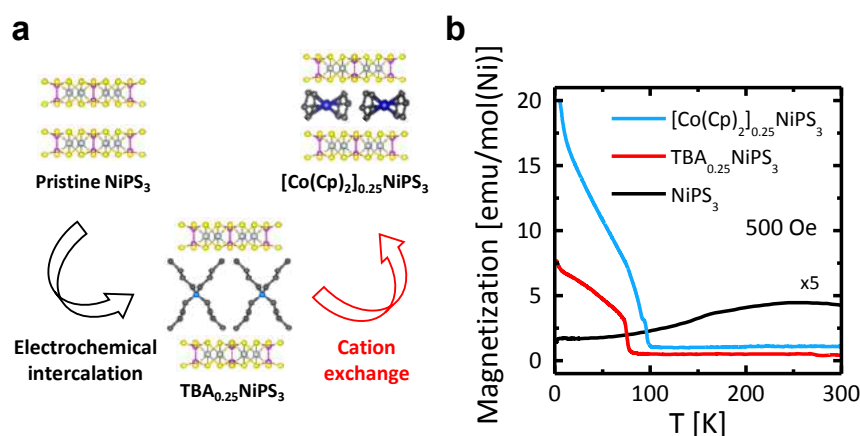


Figure 1: **a)** Schematic of the two-step intercalation process for NiPS₃: electrochemical intercalation of TBA⁺ ions is followed by a TBA⁺/Co(Cp)₂⁺ exchange; **b)** molar magnetization vs. temperature of pristine NiPS₃, TBA_{0.25}NiPS₃ and [Co(Cp)₂]_{0.25}NiPS₃.

Decoherence-free molecular spin qubits with chemically designed frequencies

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We report a sizeable quantum tunnelling splitting for the mononuclear Ni(II) molecular complexes [Ni(Me₆tren)Cl](ClO₄) (**1**) and [Ni(2-Imdipa)(NCS)](NCS) (**2**).^[1,2] With their $S = 1$ ground state and strong anisotropy, these molecules provide a realization of the simplest non-Kramers system (integer spin). The “clock transition” between levels associated with superpositions of $m_S = \pm 1$ spin states, with its characteristic non-linear magnetic field dependence, has been directly monitored by heat capacity experiments. The comparison of complex **1** with a Co derivative ($S = 3/2$), for which tunnelling is forbidden, shows that the clock transition leads to an effective suppression of intermolecular spin–spin interactions.^[3] We also show that the splitting admits a chemical tuning via the modification of the ligand shell that determines the magnetic anisotropy. In particular, the weaker magnetic anisotropy of complex **2** makes its qubit frequency compatible with superconducting microwave circuits, and has allowed its direct detection by on-chip broadband transmission experiments.

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Figures

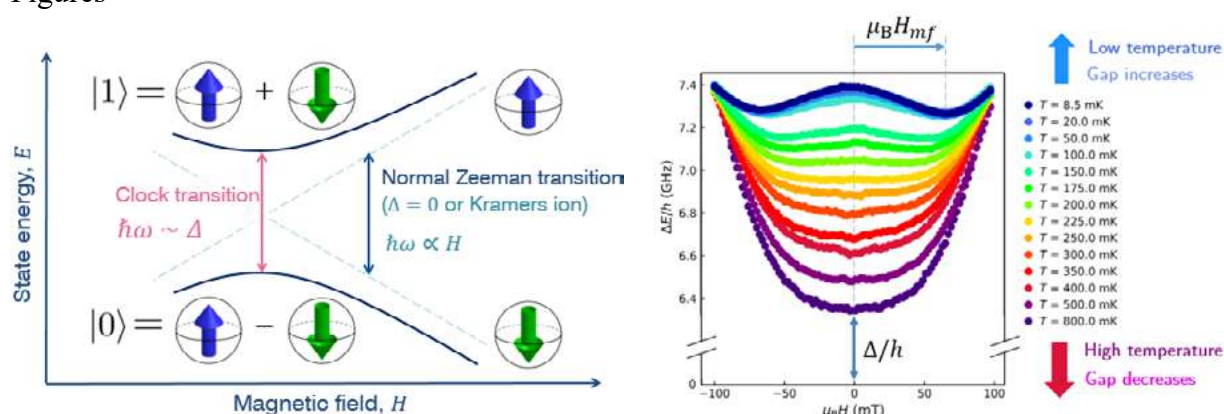


Figure 1. Left: Scheme of the clock transition in complexes **1** and **2**. The two states of the transition are superposition states of $m_S = \pm 1$ spin states. Right: Evolution of the resonance frequency of the clock transition of complex **2** with magnetic field and temperature, extracted from on-chip broadband transmission data. Thanks to the smaller gap of complex **2** compared to that of complex **1** it is possible to see a magnetic phase transition in the system through the effect of spin-spin interactions on the effective energy gap of the clock transition.

Magnetic order in a coherent two-dimensional Kondo lattice

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Kondo lattice systems are of fundamental importance for our understanding of quantum criticality and unconventional superconductivity. At the heart of their complexity lies the competition between the opposing forces of Kondo screening and magnetic interactions, which is revealed at very low temperatures as the moments start behaving coherently and eventually determines the fate of the ground state. While our understanding of Kondo lattices has traditionally relied on technically challenging strongly correlated bulk f-electron systems, new light is being shed on the problem thanks to heterostructures of 2D transition metal dichalcogenides (TMD), which realize a tunable Kondo lattice platform in a simple material. Here, we study the 1T/1H-TaSe₂ heterostructure via scanning tunneling microscopy/spectroscopy (STM/STS) at low temperatures (340 mK) to unveil the emergence of coherent magnetism in this artificial 2D KL [1]. Our measurements demonstrate spin coherence in a 2D Kondo lattice as opposed to the well-studied isolated-moment Kondo physics. Unexpectedly, we show that our system exhibits long-range antiferromagnetic order driven by indirect RKKY interactions and, more importantly, does not condense into a Kondo insulator state as commonly assumed for this type of heterostructures. The observation of coherence behavior demonstrates that long sought Kondo phenomenology can be observed in such accessible systems, drawing a pathway towards the exploration of quantum criticality, Kondo breakdown transitions, non-Fermi liquid behavior and unconventional superconductivity.

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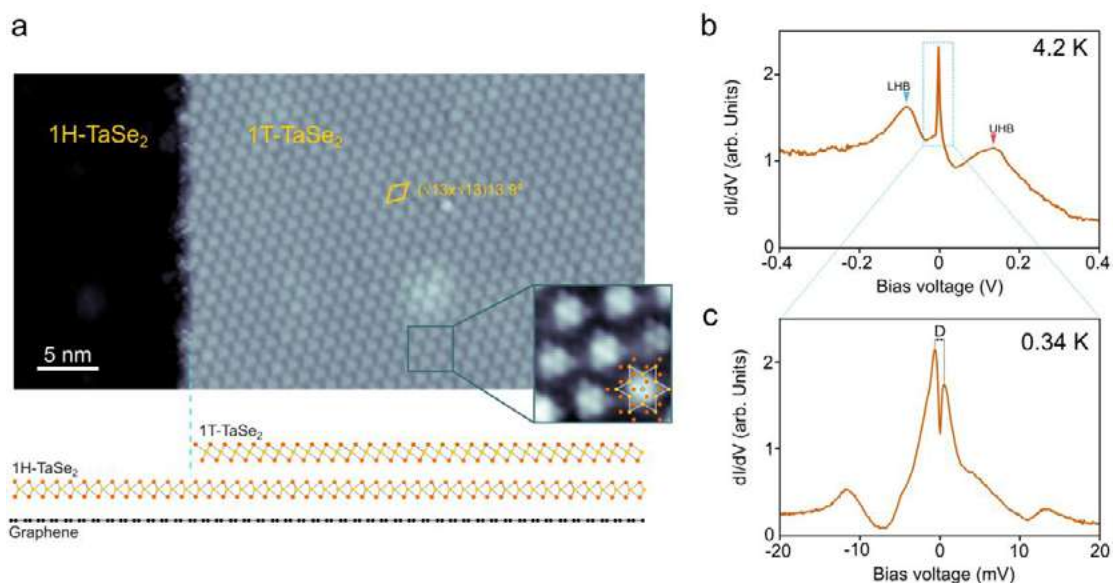


Figure 1: **a**, STM image of 1T/1H-TaSe₂. Below a sketch of the vertical arrangement of the heterostructure is shown. Se, Ta and C atoms are displayed in orange, yellow and black, respectively. dI/dV spectra taken on the 1T/1H heterostructure at 4.2 K (**b**) and 0.34 K (**c**).

Stress effects on ferroelectric doped epitaxial HfO₂ oxide films and its impact on functional properties

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11 years ago, ferroelectricity in doped Hafnium oxide was reported for the first time. From then on, a flurry of research on ferroelectric HfO₂ has been and is being carried out, because its high interest for memory applications due to its CMOS compatibility. Different strategies to stabilize and tailor the presence of the ferroelectric orthorhombic phase has been followed. These strategies involved, but are not limited to, the use of different dopants, the stress effects and the use of different capping layers. However, most of these studies are done using polycrystalline samples. Despite their appealingness from the technological point of view, fundamental understanding in polycrystalline films can be hindered by the presence of different phases, crystalline orientations and large number of defects. Epitaxial films of higher crystalline quality are then an ideal candidate for fundamental research.

I will present a general view of structural, morphological and functional properties of epitaxial films grown on perovskite substrates with state-of-the-art polarization, endurance and retention. The evolution of functional properties with films with different stress modified by the use of different substrates will be described. In short, it is found that tensile stress promotes the presence of orthorhombic phase leading to larger ferroelectric polarization but not to better endurance. These effects are observed in HfO₂ with optimal Zr and La doping (Fig. 1). The involved mechanisms will be discussed. It is also observed that films showing larger presence of orthorhombic phase show slower switching dynamics, which is contrary to what is found in archetypical ferroelectrics [1-3].

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Figures

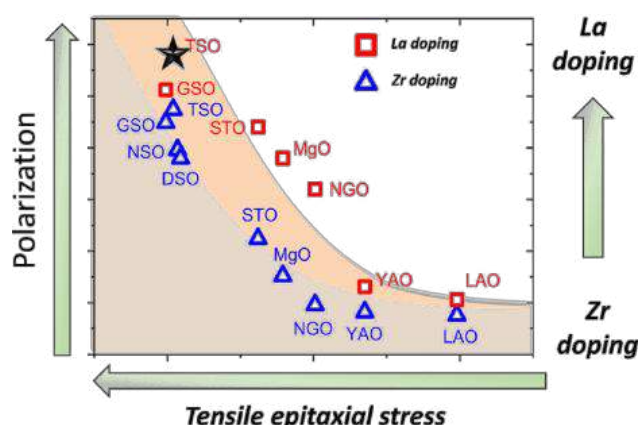


Figure 1: Dependence of remanent polarization on tensile epitaxial stress for epitaxial La and Zr doped films.

Low temperature MFM characterization of adjustable 3D ferrimagnetic NdCo/GdCo/NdCo trilayers

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Multilayered systems allow us to tune the desired magnetic behavior of the entire structure by precisely adjusting material properties, thicknesses, and magnetic interactions such as exchange and magnetostatics for the involved materials. This capability is extremely useful to build advanced spintronic devices or magnetic recording media. Ferrimagnetic materials such as Gd-Co alloys exhibit adjustable magnetization, offering the possibility of controlling features such as spin-wave modes, skyrmion nucleation or fast domain wall motion [1]. In addition, temperature dependence of all these properties increases the interest of this kind of systems.

A GdCo/NdCo/GdCo trilayered system has been designed to support an exchange spring at the top layer as ferrimagnetic GdCo alloys present a soft magnetic behavior with weak PMA [2] [Figure 1], so the middle NdCo layer with its high anisotropy (one order of magnitude larger than GdCo layer) can create a pattern of stripe domains with alternating up-down magnetization orientation, that can be used to control the configuration in the neighboring GdCo layers via interfacial exchange and magnetostatic interactions.

Low temperature MFM under variable field shows the results of the anisotropy, exchange and magnetostatic interactions across the entire GdCo/NdCo/GdCo trilayer: Stripe pattern reconfiguration along the entire hysteresis loop (mainly induced by the NdCo mid-layer) and the collapse of the top PMA stripe pattern above $B_z=800\text{mT}$.

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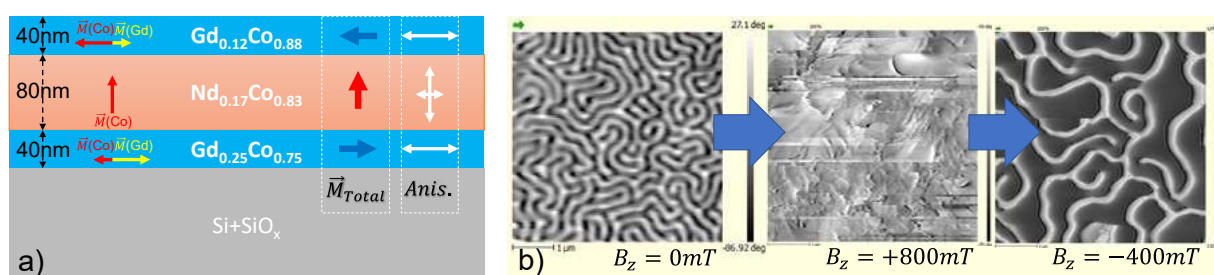


Figure 1. a) Exchange coupled GdCo/NdCo/GdCo trilayers b) MFM characterization at 4K and $B_z=0, +0.8\text{T}$ and -0.4T

Probing strain-induced ferromagnetism in epitaxial SrMnO₃ films

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The development of multiferroic materials with strong magnetoelectric coupling would allow creating low energy consumption devices where the magnetic response could be controllable by an electric field. The coexistence between magnetism and polar order — driven by the off-centering of the magnetic Mn⁴⁺ cation (d³) — has been observed in SrMnO₃ perovskite compounds [1,2]. As the same cation is responsible for both the polar and magnetic orders, strong magnetoelectric coupling is expected. While in bulk SrMnO₃ the Mn — O — Mn superexchange magnetic interaction stabilizes the G type antiferromagnetic (AF) order, first-principles calculations suggest that different magnetic ground states may be accessible in SrMnO₃ epitaxial films by tuning the biaxial strain exerted by the substrate [3,4]. For tensile stress, a rich phase diagram is inferred, in which a progressive increase in the strain magnitude induces a gradual transition from different types of AF orders to eventually a ferromagnetic (FM) order [3,4].

Here, we study three fully strained 10 nm-thick SrMnO₃ epitaxial films grown on (La,Sr)(Al,Ta)O₃ (LSAT), SrTiO₃ (STO), and DyScO₃ (DSO) single-crystal substrates with mismatch values of +1.68%, +2.63%, and 3.78%, respectively, in order to determine the strain-oxygen vacancies-magnetic phase diagram. Synchrotron-based X-ray linear dichroism (XLD), X-ray magnetic circular dichroism (XMCD), and element-specific magnetic hysteresis loops, were performed in all samples around the L_{2,3}-Mn edges at low temperature and high magnetic field. Preliminary results show sizeable XMCD signals and a slight opening of the hysteresis loops in the case of the DSO and LSAT, suggesting the emergence of FM order in these strained systems (see Figure 1). Besides, the comparison of the experimental data with calculated reference spectra is also in progress to determine the evolution of the Mn³⁺/Mn⁴⁺ ratio as a function of the strain and its effect on both the local magnetic moment and the resulting magnetic order.

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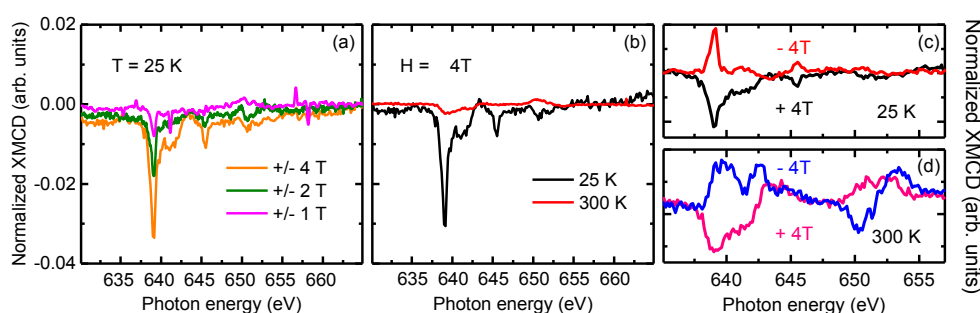


Figure 1: XMCD for the SrMnO₃ thin film grown on DSO. (a) Magnetic field dependence. (b) Temperature dependence. Panels (c) and (d) depict inversion of the signal with opposed magnetic fields.

Low dimensional effects in artificial spin ices and superconducting nanostructures

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New emergent phenomena arising from topological effects have become a very active research frontier in condensed matter physics. Artificial spin ices (ASI) are examples of magnetic interacting nanostructures which have opened a way to study topological phenomena such as frustration, emergent magnetic monopoles and phase transitions. Geometric properties of the ASI are key to determine the dynamics of the magnetic charges and the possible energetic configurations, which can also have an influence on the magnetic textures present in these systems. Additionally, due to the miniaturization of electronic devices, quantum mechanical effects become important. Another interesting effect is how the collective properties of these devices, such as superconductivity, are affected when the systems dimensions are reduced. In this context, low dimensional effects in superconducting nanostructures have been studied.

The main goal of this work is to characterize the magnetic properties, spin textures and frustration in ASIs with different geometries and its influence in the formation and ordering of magnetic features. ASIs with different geometries and types of topological protection will be presented. Furthermore, this work study how the fabrication process of superconducting nanostructures based on a single hexagonal ASIs vertex influences the superconducting properties.

Different geometries of ASI systems and superconducting nanostructures had been fabricated by combining nanolithography techniques (optical and electronic lithography) and DC magnetron sputtering. Nanostructures were characterized using different microscopy techniques (AFM and SEM), magnetic force microscopy (MFM) (Fig.1) and micromagnetic simulations. Additionally, transport measurements of the superconducting nanostructures at low temperature allows the distinction of two different regimes due to lateral confinement: nanowire regime and thin film regime.

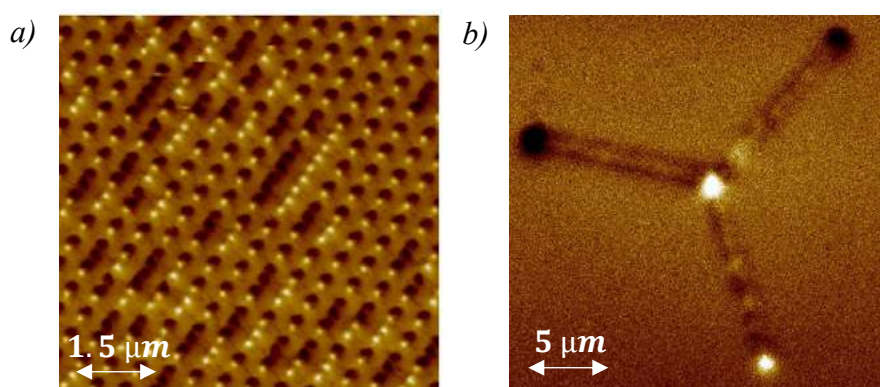


Figure 1: MFM images of a) square artificial spin ice. b) single vertex of hexagonal artificial spin ice.

Certifying entanglement of spins on surfaces using ESR-STM

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We propose a protocol to certify the presence of entanglement in artificial on-surface atomic and molecular spin arrays using electron spin resonance carried scanning tunnel microscopes (ESR-STM) [1]. We first generalize the theorem that relates global spin susceptibility as an entanglement witness [2] to the case of anisotropic Zeeman interactions, relevant for surfaces. We then propose a method to measure the spin susceptibilities of surface-spin arrays combining ESR-STM with atomic manipulation [3]. Our calculations show that entanglement can be certified in antiferromagnetically coupled spin chains with an odd-number of spins using state of the art spectral resolution of ESR-STM magnetometry.

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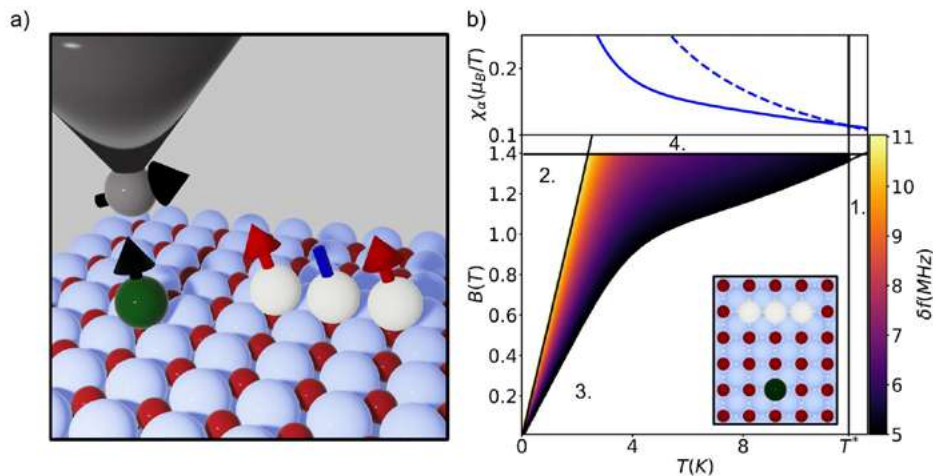


Figure 1: a) Main elements of the proposed protocol: a spin-polarized STM, an ESR-STM active adatom (green), and the spin structure (white) for which entanglement is certified. b) Top, spin susceptibility and the entanglement witness boundary for entangled states (solid and dashed blue lines respectively) for an antiferromagnetic spin trimer with $J = 1$ meV. The bottom panel shows the entanglement certification window as the area in the B, T plane inside these four regions with the imposed limitations: 1. Limit temperature for entanglement (T^*). 2. Linear response regime of magnetization of the spin chain with the external magnetic field. 3. Resolution limit of the ESR-STM sensor, 4. Limit of the excitation bandwidth of ESR-STM. The position of the sensor is at three oxygen lattice distances in MgO (inset).

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In-situ characterization of NMC particles with applications in Li-ion batteries

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The advent of modern Lithium-ion batteries (LiBs) and energy storage technologies will rely on innovative materials and improved characterization techniques in the search of high-energy and long-term cycling LiB components [1, 2]. Amongst the most promising materials used as cathodes, Ni-Mn-Co (NMC)-based compounds with core-shell structure are gaining increased attention owing to their high specific capacity and thermal stability. The characterization of these materials requires of advanced microscopy and spectroscopy techniques, including *in-situ* and *in-operando* techniques, in order to achieve deeper comprehension of the phenomena governing the battery performance.

In this work, NMC core-shell microparticles have been studied by a combination of techniques including scanning electron microscopy (SEM), X-ray diffraction (XRD), thermo-XRD, energy dispersive x-ray spectroscopy (EDS), Raman spectroscopy, and X-Ray Photoelectron Spectroscopy (XPS), including *in-situ* characterization as well. The combination of these techniques allows to achieve insights in the morphological, structural, compositional, and electronic properties of the NMC microparticles under study. The analysed microparticles exhibited a rounded appearance with an average diameter of 4 μm and variations in their morphology and properties as a function of the synthesis route, as observed by SEM and XRD. The presence of Ni-rich core and a Mn-rich shell with submicrometric dimensions have been confirmed by EDS, while the formation of oxides presenting the usual layered structure of NMC (R-3m) together with the appearance of spinel phases as a function of the synthesis procedure have been assessed by means of XRD and Raman spectroscopy. This layered structure is directly related to the high capacity and structural stability of NMC cathodes when the battery is cycled. Further characterization, including *in-situ*-thermo XRD, *in-situ* XPS under variable pressure, as well as *in-situ* SEM with variable temperature up to 900 °C have been also carried out. These measurements confirm the formation of NiO as the temperature increases up to 900 °C, as well as the promotion of changes in the morphology of the microparticles. Finally, *in-situ* XPS measurements at temperatures up to 500 °C and a variable pressure, indicate variations in the Mn(3s) and O(1s) core levels, as well as in the electrical conductivity of the samples. The combination of these results, including the *in-situ* characterization, can lead to achieve a deeper knowledge of the properties of the NMC microparticles in the search of improved performance in LiBs.

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Layer-dependent evolution of the optical properties in 2D CrI₃ mapped by hyperspectral imaging

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Magnetic 2D materials have been recently attracting a pivotal attention thanks to both fundamental breakthrough studies in low-dimensional magnetism [1] and device applications [2]. The potential to fabricate ultra-thin magnetic devices paves the way to change the miniaturization paradigm of the limitations of magnetic-enabled microelectronics and integrated photonics [3]. However, the integration of these materials in photonic devices requires an accurate determination of the optical properties down to the monolayer limit [4], which is still missing. By using hyperspectral wide-field imaging we acquire transmission spectra of mechanically exfoliated CrI₃ flakes with different thickness (Figure 1). We extract the complex dielectric function by modelling the spectral information using a Drude-Lorentz model as a function of the layer number and relying on a simultaneous fit of a large number of spectra of different thickness to increase the consistency of our analysis. Our results reveal a non-monotonic layer-dependent evolution of the optical properties that extends across different length up to mesoscale (> 100 layers). These results shed light into the open structural conundrum of this material and will advance the understanding and manipulation the magneto-optical effects of magnetic 2D materials for future applications.

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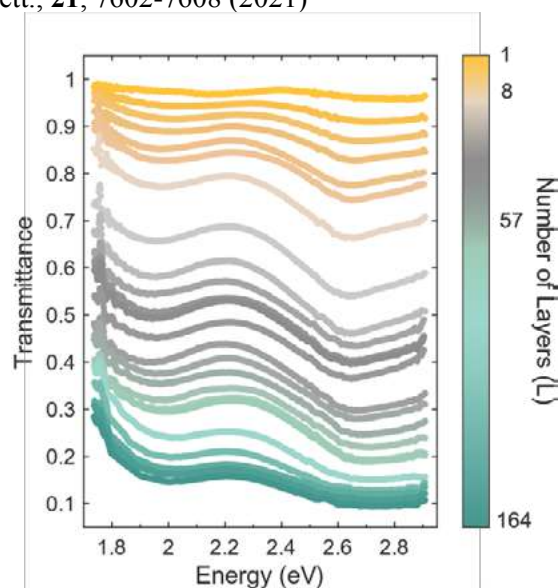


Figure 1: Visible range transmittance spectra of CrI₃ crystals. Absorption features visible at about 1.95 eV and 2.7 eV present a non-monotonic trend with the number of layers.

Dislocations in GaN on sapphire for power applications: an ultraviolet light-assisted Kelvin probe force microscopy study

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Wide band gap materials such as gallium nitride (GaN) have attracted great interest due to their potential to improve the performance of power electronic devices. When compared with other semiconductors, GaN-based vertical devices can operate at higher temperatures and have a larger critical field or a larger blocking voltage, among other advantages. [1] Nevertheless, GaN usually bears a high density of structural defects, such as dislocations which can compromise the reliability of GaN-based devices. Therefore it is important to obtain information of the growth-induced dislocations and their effects in the electrical properties of the material. Kelvin probe force microscopy (KPFM) is presented as a non-invasive technique that can address this challenge.

In this work, light-assisted KPFM is used for the characterization of the dislocations in two GaN multilayer samples (S1 and S2) grown by Metal Organic Vapor Phase Epitaxy on 100 mm diameter c-plane sapphire substrates. The atomic force microscopy characterization shows a similar topography in both samples: terraces characteristic of step-flow growth containing defects, most commonly in the form of pits. The observed defects present three different behaviors concerning contact potential difference (CPD) value and its change upon above band-gap illumination (325 nm, UV). First, those appearing as large pits (~90 nm diameter) assigned to open core dislocations present larger CPD values on their surrounding area. Upon UV illumination, the contrast disappears. Smaller pits (~65 nm diameter), assigned to pure screw dislocations, do not show any special CPD contrast. And finally, mixed dislocations do not show any CPD features before illumination. Under UV illumination, we observe a local drop in the CPD that persists for several hours after placing the sample in the dark. Mixed and pure dislocations are mainly present in S1, while open core dislocations are observed in S2. Figure 1 shows the topography (a) and CPD (b) ascribed to mixed and pure screw dislocations of S1. In (c) we have represented the time evolution of the surface photovoltage of both defects.

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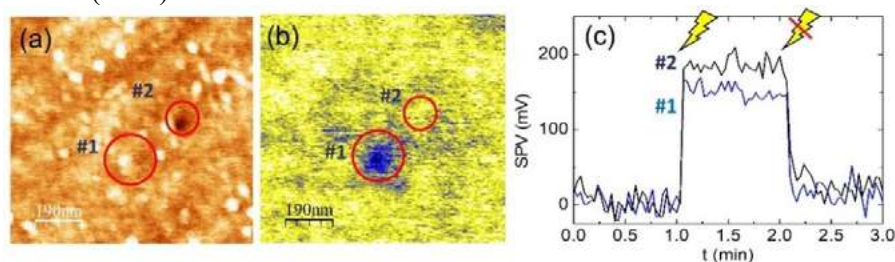


Figure 1: (a) S1 topography (scale from 0 to 2 nm, RMS 0.3 nm). (b) Light assisted KPFM (CPD scale from 710 to 910 mV). Red circles show mixed and pure screw dislocations, #1 and #2 respectively. (c) SPV vs. time when light is turned on and off (time resolution 2 s).



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Magnetic Domain Wall Ferromagnetic Resonance Confirmed by Magnetotransport Measurements and Kerr Microscopy

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In spintronics application, the generation and manipulation of magnetic domain walls have been an important research field since its proposal as key element in magnetic data storage structures [1]. Nowadays, this systems are studied, not only for its information storage capabilities, but for its potential application to process such information in a computational way with low energy consumption [2, 3], apart from the generation of microwave signals [4]. In this work we show ferromagnetic resonance of the magnetization of a permalloy microstrip with a gold microantenna sputtered over it, measured by the stripline ferromagnetic resonance technique [5]. The behavior of the microstrip resonance with the radiofrequency stimulus and the applied magnetic field fits the Kittel's equation. A new resonance is observed between 4 Oe and 9 Oe for an applied radiofrequency signal from 2.0 GHz to 3.0 GHz approximately. Throughout magnetoresistance measurements, this new resonance at low magnetic fields was found to correspond to the formation and pinning of a magnetic domain wall. The presence of the domain wall was confirmed by Kerr microscopy.

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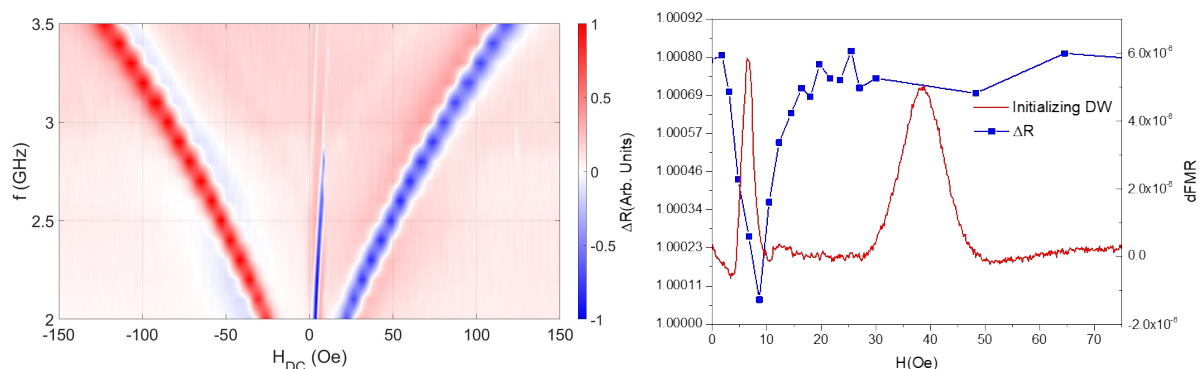


Figure 1: Normalized measurement of the derivative of ferromagnetic resonance signal from 2.0 GHz to 3.5 GHz at 0 dBm and the shape anisotropy axis of the sample oriented at 0° with the applied magnetic field (left). Derivative of ferromagnetic resonance in red line, and simultaneous magnetoresistance measurements in blue dot and line representation at 2.3 GHz (right).

A Versatile 3D Printable Scanning Tunneling Microscope

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Here, we propose a new and versatile prototype of a 3D printable Scanning Tunneling Microscope. In our prototype (see figure 1), the most important advantages that we introduce are: the price of the manufacture, a standardized product, and the quickly interchange between different approaches, such as STM topography and STM in Break Junction approach (STM-BJ). Our results obtained via finite elements simulations have demonstrated that the mechanical stability of STM manufactured with poly lactic acid (PLA) is comparable with the conventional manufacturing materials. Moreover, we have demonstrated that full functionality of this prototype via STM images and electronic transport experiments (STM-BJ).

Thanks to the versatility offered by the 3D printer, we have developed a novel technique based on the combination of scanning tunnelling microscopy and twistronics, which we call Twisted STM in break junction approach (Tw-STM-BJ). This new technique allows to afront the STM electrodes by their 2D edges and change the relative angles between them [ref.1].

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Figures

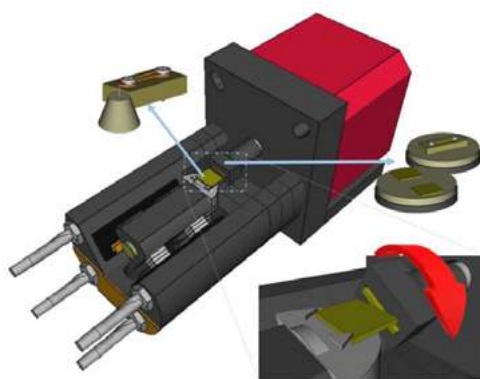


Figure 1: Illustration of the microscope together with its accessories, which allow interchange between STM, STM-BJ and Tw-STM-BJ experimental techniques.

Observation of an anisotropic two-dimensional electron gas at the (110) surface of KTaO_3

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In 2004, a high mobility two-dimensional electron system (2DES) was found at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface [1]. Later on, an intense effort in the oxide electronics community was started to gain insight into the underlying physics of complex oxide-based 2DESs, as well as into the experimental procedures for creating such systems [2,3]. Recently, an especial focus was placed in KTaO_3 -based 2DESs for two reasons. Firstly, the large spin-orbit coupling increases the Rashba spin-splitting, which results in exciting and feasible applications in spintronic devices [3]. Secondly, anisotropic transport properties and superconductivity for the $\text{KTaO}_3(111)$ and (110) 2DESs were recently observed [4]. Remarkably, superconductivity has never been seen before in bulk KTO crystals. In this context, we show for the first time ARPES measurements of the 2DES formed in $\text{KTaO}_3(110)$. Our experimental results are in good agreement with the band structure simulations that we performed using an open-source code that we have developed [5]. By changing beam polarization and analyzing the matrix element symmetries, we have elucidated the strong anisotropy of the band structure. Based on our band-structure simulations we will discuss the orbital-ordering and spin texture in KTO based 2DES which are of great interest for the spintronics community.

Acknowledgments:

This work has been supported by Comunidad de Madrid, Spain (Atracción de Talento grant No. 2018-T1/IND-10521) and by MICINN, Spain PID2019-105238GA-I00.

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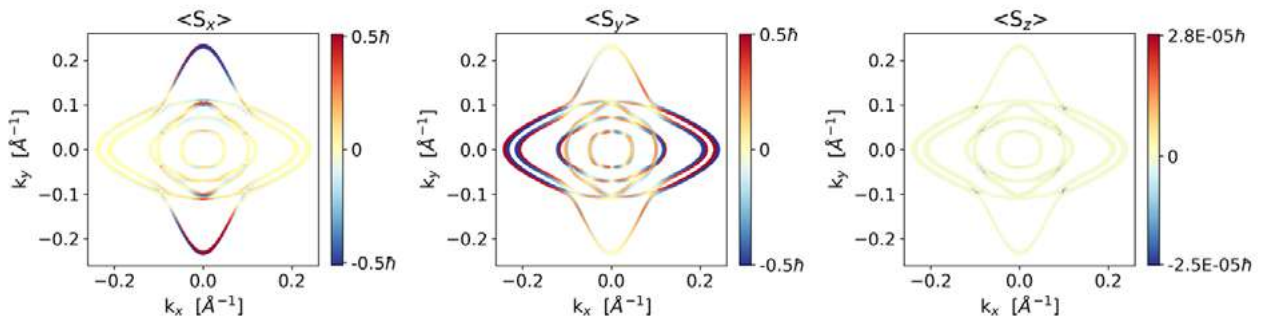


Figure 1: Spin expectation values computed for the Fermi surface of the $\text{KTaO}_3(110)$ two-dimensional electron system.

Atomic resolution studies of low dimensional Bi-doped Cu nanowires for spintronics applications

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The spin Hall effect (SHE) is an important spin-charge conversion mechanism that plays a key role in the development of spintronics devices [1], so the search for materials that exhibit giant SHE constitutes a quite active research field [2]. Large spin Hall angle (SHA) has been reported [3] in CuBi alloys with Bi contents around 0.5%, making this material a good candidate for integration in spintronics devices. For this idea to be realized, a detailed study of the structure and a fine control of composition and crystal quality is a must so a deeper understanding of the origin of extrinsic SHE in this material can be achieved.

In a previous work we reported the possibility of obtaining Bi-doped Cu nanowires using template assisted electrochemical deposition [4]. This growth method allows the independent control of factors such as crystal quality, cluster formation or microstructure. In this work, we present an extensive atomic resolution scanning transmission electron microscopy (STEM) characterization of this material. Preliminary TEM structural characterization reveals that using low overpotential results in growth of single crystal nanowires (Figs 1 a,b). For low doping levels, Bi does not cluster but instead it appears homogeneously distributed into the Cu matrix, as Fig 1c shows. These results proof that the obtention of single crystal, homogeneously doped wires is indeed possible. This is a much needed step to enable future studies on the correlation between the structure and the spin-transport properties to pave the way towards a future understanding of the large SHE in these systems.

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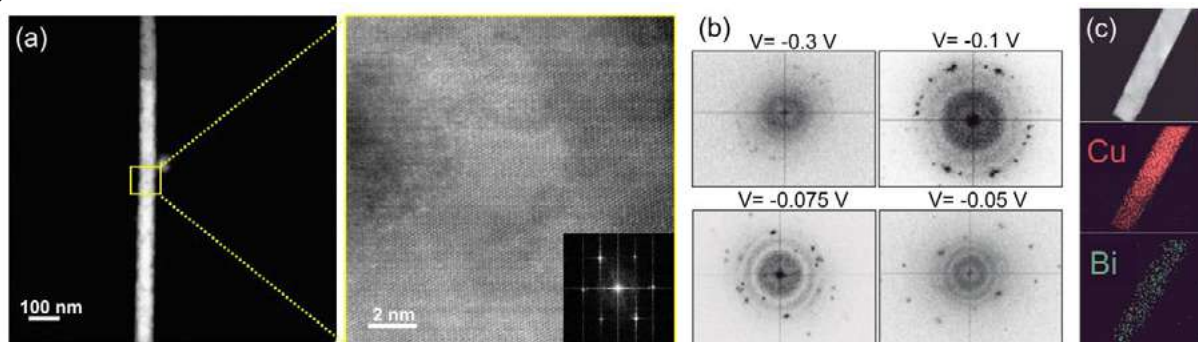


Figure 1: (a) High-angle annular dark field STEM images corresponding to a single-crystal nanowire (NW) with composition $\text{Cu}_{95}\text{Bi}_5$ grown at -0.05 V. Bottom right inset shows the fast Fourier transform in the zone axis $[100]$. (b) Selected area electron diffraction patterns measured for NWs grown at different overpotential. (c) Energy dispersive X-Ray analysis maps measured for Bi and Cu of the simultaneous TEM image.

Synthesis and Characterization of Magnetic Aza-Triangulene Nanostructures

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The emergence of spin states in triangular-shaped graphene fragments with zig-zag edges (triangulenes) is a conceptually attractive theoretical proposal from decades ago ^[1]. Thanks to the recent development of on-surface synthesis strategies, triangulene nanostructures showing magnetic interactions can now be fabricated on metal substrates with atomic precision ^[2].

In this work, we present the synthesis and characterization of aza-[5]-triangulene (A5T) ^[3] and π -extended-aza-[5]-triangulene (eA5T) ^[4] on Au(111) surface. Theoretical models predict such structures to have more than two unpaired electrons, which could result in large spin states and magnetic interactions. Combined low temperature scanning tunnelling microscopy (LT-STM), and low temperature atomic force microscopy (LT-AFM) measurements using CO-functionalized tips confirm the precise structure of the triangular flakes. Scanning tunnelling spectroscopy (STS) was used to directly prove the magnetic character by measurements of the Kondo effect and spin excitations. Experimental findings are further corroborated by the predictions of theoretical models such as density functional theory (DFT), mean-field Hubbard model (MFH), and complete active space (CAS) Hubbard model. The N heteroatom substitution modifies the spin ground state of the molecules with respect to their undoped counterparts, while the size extension switches from ferromagnetic to antiferromagnetic interaction between the radicals.

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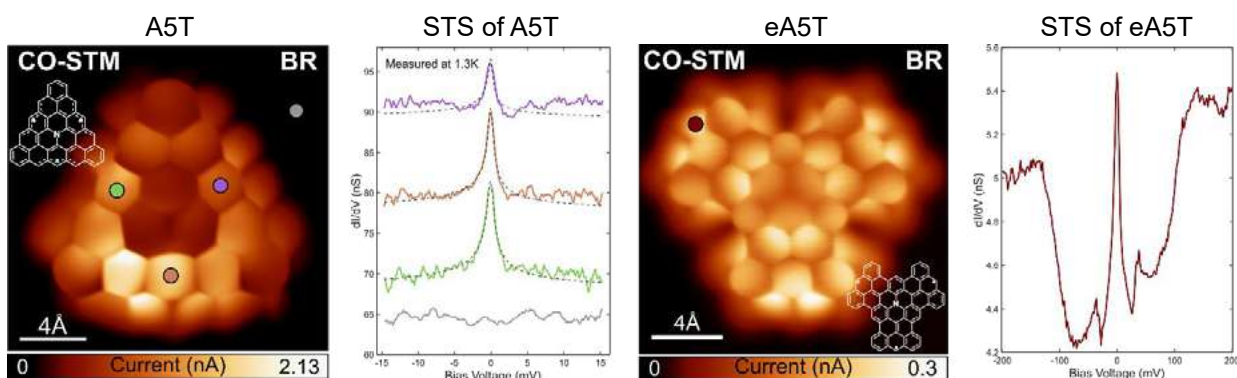


Figure 1: Bond-resolved images with CO-STM of A5T and eA5T showing the chemical structures as insets and the spots where STS spectra were recorded. STS of A5T shows a weak Kondo resonance corresponding to a high spin ($\geq 3/2$) ground state. STS of eA5T shows a sharp and intense Kondo resonance corresponding to spin $1/2$ ground state and inelastic doublet-quartet spin excitations.

Angle Resolved Reflection Electron Spectroscopy in a Low-Energy Electron Microscope: the path to map the unoccupied states in the Nanoworld

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The electronic structure of materials is crucial for our understanding of their properties. In crystalline materials, including 2D materials, the occupied states are now routinely determined by Angle Resolved Photoemission Spectroscopy. Until now, the main techniques for the equivalent mapping of unoccupied states have been either Inverse Photoemission Spectroscopy or Two-Photon Photoemission Spectroscopy. However, both techniques have complications that severely limit their application in practice. Instead, with the availability of Low-Energy Electron Microscopes (LEEM), the use of elastically scattered electrons to probe the unoccupied density of states has been proposed by van der Molen and coworkers[1], in what has been denoted Angle Resolved Reflection Electron Spectroscopy (ARRES). Furthermore, if a spin-polarized electron source is available, the spin-resolved ARRES map can be acquired. We have recently started to acquire (ARRES) maps on several materials. We will present results on clean surfaces such as Ru(0001), 2D materials as well as in highly correlated oxides such as magnetite, both from bulk crystals and from nanostructures. The experiments have been performed at the LEEM instrument in the Instituto de Química Física “Rocasolano” in Madrid, and at the spin-polarized LEEM microscope in Lawrence Berkeley National Laboratory. Both instruments are open to members of the Spanish scientific community and researchers abroad.

Acknowledgments

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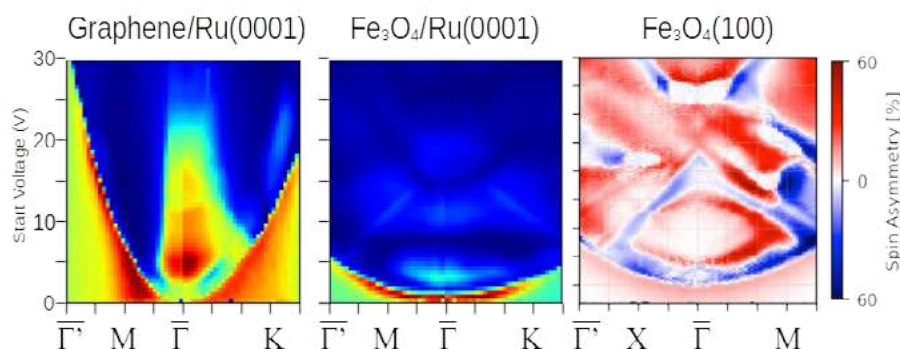


Figure 1: ARRES maps of graphene, a magnetite island on Ru(0001) and magnetite(100) (the latter spin-resolved).

Electronic band structure of the Co pnictide $A(\text{CoX})_2$ ($A=\text{Ca, Eu}$ and $X=\text{As, P}$) probed by ARPES

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The pnictide family of transition metals is being widely studied for emergence of new collective quantum states. In the iron-family, the suppression of the antiferromagnet order is accompanied with the emergence of superconductivity [1] and the Ni-based family has been demonstrated to show an electronic liquid nematic ground state [2]. The Co-pnictide family (ACo_2X_2 , $A=\text{Ba, Ca, Eu, ...}$ $X=\text{As, P}$) has been discussed in the framework of itinerant magnetism of conducting electrons and non-Fermi liquid scenarios. Besides, some of these Co-pnictides have been predicted to be topological Weyl semimetals where the low-energy excitations are Weyl fermions [3]. The experimental observation of these surface states gives an unequivocal proof that a particular compound is a Weyl semimetal [4]. Here, by means of ARPES and DFT, we report the experimental and theoretical band structure of the magnetic Co-pnictide ACo_2X_2 ($A = \text{Ca, Eu}$ and $X = \text{As, P}$). We address the role of the dimensionality, disorder and the possible observation of topological physics.

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A Laser-ARPES View of the 2D Electron Systems at LaAlO₃/SrTiO₃ and Al/SrTiO₃ Interfaces

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The electronic structure of the two-dimensional electron system (2DES) found at the Al/SrTiO₃ (Al/STO) and LaAlO₃/SrTiO₃ (LAO/STO) interfaces is measured by means of laser angle resolved photoemission spectroscopy (ARPES), taking advantage of the large photoelectron escape depth at low photon energy to probe these buried interfaces. The possibility of tuning the electronic density in Al/STO by varying the Al layer thickness is demonstrated,[1] paving the way for a designed band structure in devices. A new open source Python code released under the name *BinPo* is used to compute the electronic structure of the 2DES. [2] We show that the electronic structure evolution for different densities differs qualitatively from a rigid band shift model. A comparison of the ARPES measurements in LAO/STO and Al/SrTiO₃ allows us to shown that both 2DES are strongly coupled to longitudinal optical phonons, in agreement with previous reports of a polaronic ground state in similar STO based 2DESS.[3] Tuning the electronic density in Al/STO to match that of LAO/STO and comparing both systems, it is estimated that the intrinsic LAO/STO 2DES has a bare band width of ≈ 60 meV and a carrier density of $\approx 6 \times 10^{13} \text{ cm}^{-2}$. [1]

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Figures

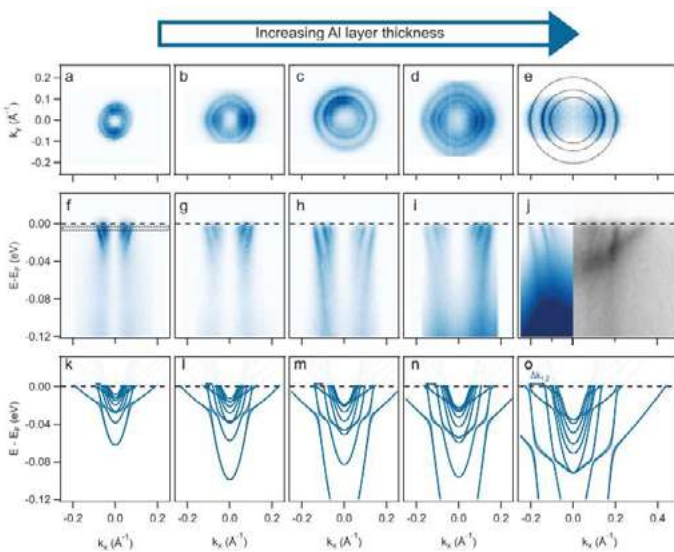


Figure 1: (a-e) ARPES Fermi surface of the 2D electron system stabilized at the Al/SrTiO₃ interface for increasing Al thickness. These plots are obtained by summing two measurements with s and p polarization, respectively, and integrating the spectra within an energy window of ± 5 meV around E_F . f-j) Energy-momentum dispersion measured along the [100] high symmetry direction ($k_y = 0$). The right half of panel (j) shows synchrotron data acquired in the second Brillouin zone with a photon energy of 52 eV on a bare STO surface cleaved in UHV. All other data on Al/STO were acquired in the first Brillouin zone with $h\nu = 6$ eV. (k-o) Self-consistent tight binding supercell calculation of the electronic band structure. The electronic densities are from first to last column: 6, 10, 14, 17, and 31 (10^{13} cm^{-2}).)

Magneto-transport properties and anomalous Hall effect in ferromagnet/nanostructured superconductor hybrid systems

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Ferromagnetism and superconductivity are still attracting a lot of attention in the condensed matter physics community not only due to the rich physical phenomena they embrace but also due to their great potential in different novel applications (memories, sensors, quantum devices...). Although they are considered antagonist effects, the interplay between them can lead to a wide variety of exotic phenomena. Some examples are superconducting vortex pinning induced by magnetic nanostructures [1], domain wall superconductivity [2], triplet superconductivity [3] and superconducting vortex – magnetic skyrmions interactions [4,5].

Here, we study magneto-transport properties of a ferromagnetic (FM) multilayer with perpendicular magnetic anisotropy (PMA) in contact with a nanostructured superconductor (SC). The magneto-resistance and Hall resistance of the FM change below the transition temperature of the nanostructured SC even when an insulating layer is placed between both materials. The symmetry of the Hall response indicates that these changes are not due to topological effects but possibly caused by modifications of magnetic structures or proximity effects.

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Exploring current limits without damaging nanostrips

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Joule heating is an undesirable byproduct in most of spintronic devices, such as nanostrips, when high current densities are delivered through them [1]. This effect must be considered in spintronic discussions as magnetic configuration can be modified by thermal gradients [2,3]. Recently we published a work proposing a method to dissipate heat by coating the nanostrip with a good thermal conductor [4]. Simulations showed a drop of 300 K in the temperature reached by coated strips in comparison with non-coated ones. This drop is higher than measuring in cryogenic conditions, method widely use in this field.

The aim of this work is to test experimentally this method covering the nanostrip with a Gold layer to dissipate heat and an insulator to avoid current leakages. We have seen that coated strips can stand higher current densities up to $3,5 \cdot 10^{12}$ A/m² of sub-microsecond pulses (Fig 1a), meanwhile non-coated stripes get damaged with current densities of $1,5 \cdot 10^{12}$ A/m². Figure 2 shows that not only higher current densities but higher temperatures can be reached with this coating layer. This layer is not just dissipating heat but giving a structural protection to the nanostrip. To the best of our knowledge, these current densities have not been seen before, so they are going to open a gate to new physics exploring the 10^{13} A/m² range.

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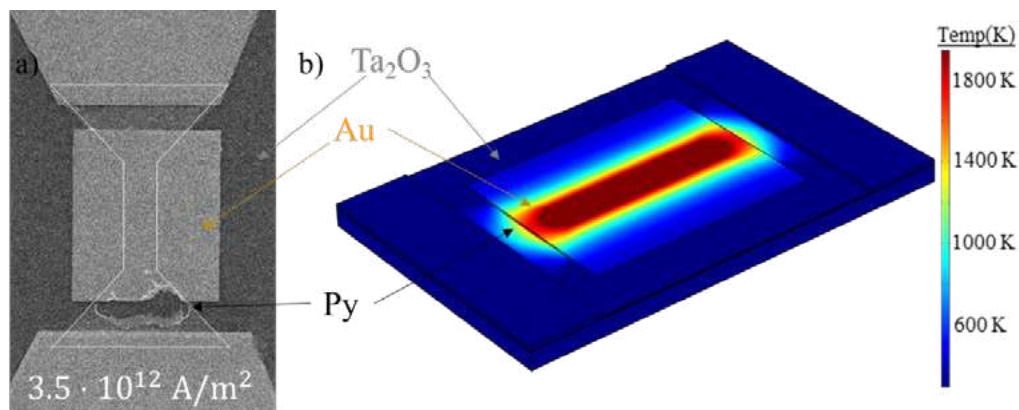


Figure 1: Scanning Electron Microscope (SEM) diagram of a damaged Permalloy strip at $3,5 \cdot 10^{12}$ A/m² (a). Temperature reached in the damaged strip (b). The different layers of the coating are shown in both figures.

Characterization of superconductivity in Full-Shell Al/InAs Nanowires

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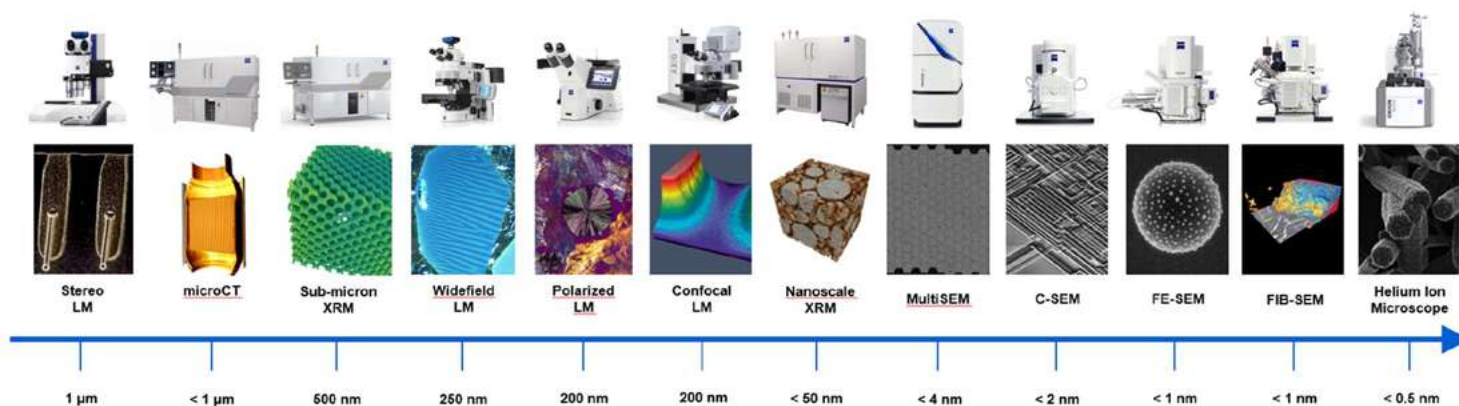
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Topological superconductivity has become a fast-growing field in the past decade following theoretical proposals [1, 2, 3] which have outlined experimental routes towards the realization of Majorana fermions [4], as well as potential applications in quantum computation [4]. InAs nanowires covered by epitaxially grown Al shells have become one of the most studied platforms in this context [6, 7, 8, 9, 10], benefitting from the improved superconducting proximity effect resulting from the high-quality material interface. Despite the significant role that the superconducting shell plays in these experiments, there are few works that fully characterize it [11]. In this work, we perform a detailed characterization of the superconductivity of the Al shell in full-shell Al/InAs nanowires. To this end, we employ DC transport to probe the resistance of the superconducting shell in different conditions of magnetic field and temperature, also in the Little-Parks regime, as well as in the presence of microwaves. Our results show a complex behavior which points towards the formation of normal regions in the superconducting shell for increasing temperature or perpendicular magnetic fields.

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Competition of Superconducting and Coulomb Correlations in Pb islands on graphene

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Superconducting and Coulomb correlations naturally compete since they induce respectively attractive and repulsive interactions. In fact, it is known that superconductivity is suppressed when the Coulomb gap is greater than the superconducting gap Δ [1,2]. The way Coulomb correlations affect superconductivity when the two energy scales are comparable remains still largely unexplored.

Here we study Pb islands [Fig1a] grown on SiC graphene by means of Scanning Tunneling Microscopy. Pb islands with lateral size $l > 100$ nm show a fully developed superconducting gap well described by BCS theory. With $l < 100$ nm Pb islands a Coulomb gap opens [Fig1b] and can coexist with the superconducting gap. In this regime we observe a strong induced asymmetry in the quasiparticle peaks that we correlate with the excess charge present on the island.

The Pb islands-substrate coupling allows controlled island lateral manipulation. Using this, we build different structures and explore how the induced superconductivity in graphene [Fig1c].

Our results show that superconducting graphene is a fascinating workbench for studying proximity effects in graphene and interplay of Coulomb blockade effects and superconductivity.

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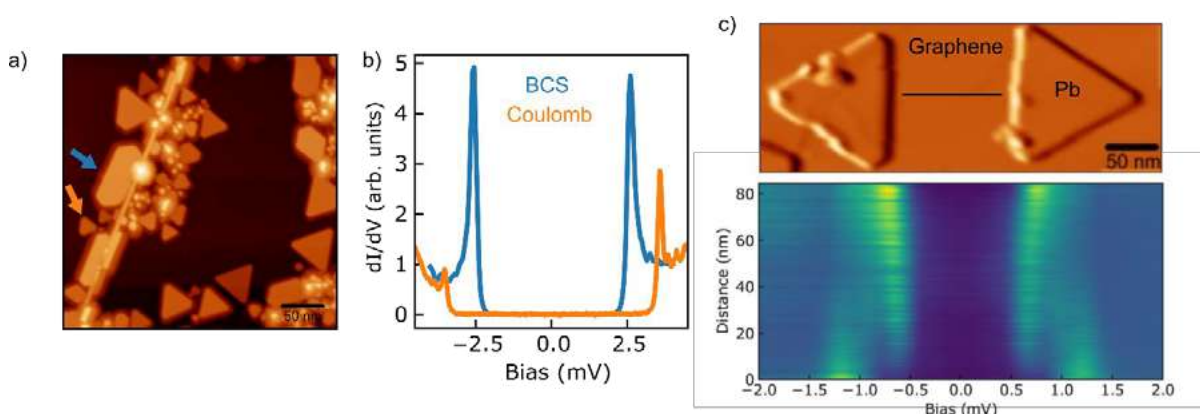


Figure 1: a) STM topography of Pb islands on graphene. B) Spectroscopy data showing density of states of the small and large islands highlighted in a). The small island shows a Coulomb gap larger than the superconducting gap. c) Resonator built with island manipulation, below a line of spectra between the islands showing the density of states in graphene.

Rapid synthesis by Joule heating of low-dimensional transition metal oxide materials

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The deviation in the properties of nanostructured materials results as well from the reduced size and/or dimensionality of the nanometer-sized crystallites as from the numerous interfaces between adjacent crystallites. Transition metal oxides represent a large family of materials possessing various interesting properties for multiple applications like electronic devices among others. Furthermore, decreasing dimensionality from bulk to nanomembranes, nanowires or nanoparticles expands the fundamental research in physics of condensed matter and the applications field.

In this work, we show a rapid synthesis method to produce transition metal oxide nano- and microstructures via the resistive heating of a metallic wire through an electric current flow in which the electromigration effect is exploited [1]. This type of synthesis has already been demonstrated as an effective route to obtain layered materials with van der Waals (vdW) bonds as MoO₃ and non-layered materials with non-vdW bonds as WO₃ [2]. The growth mechanism is based on electromigration processes that takes place due to the electric current flow through the material and promoting the ion diffusion related to thermal gradient in the wire, a characteristic process of the Joule heating [3]. Simultaneous COMSOL simulations have been carried out to verify the experimental results. Additionally, it has been studied the influence of applying an external electric field in the internal process of the growth during resistive heating. The innovation of this synthesis method is that we are capable of synthesizing different crystalline structures, including flakes, membranes and nanospheres, at the same time (depending if the growth takes place over the wire or the material deposited on the electrodes because of the electric fields' action) in a very fast and simple way. The work includes a detailed morphological, structural and chemical analysis by means scanning electron microscopy (SEM), Raman spectroscopy, X-ray diffraction (XRD), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). The last step in our investigation has been the study of the optical properties of nanostructures and composites have been elaborated, embedding the nanostructures in a poly(vinyl alcohol) matrix. In summary, the results obtained show that resistive heating is a simple method to synthesize wide-bandgap oxide nanomembranes in a fast and low-cost way with promising applications.

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Magnetic molecule as a parity sensor in entangled spin and YSR excitation on a superconductor.

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A magnetic molecule coupled to a superconductor induces Yu-Shiba-Rusinov (YSR) bound states, detected by tunneling spectroscopy as long-lived quasiparticle excitations inside the superconducting gap [1]. The degeneracy of the system can be lifted by intrinsic magnetic anisotropy so that entangled spin and YSR excitations are possible [2]. We tune the exchange coupling between a FeTPP-Cl molecule and the proximitized Au/V(100) substrate to go through a Quantum Phase Transition (QPT) from a unscreened half-integer spin (even parity) system to a screened integer spin (odd parity) system [3]. We use a single site superconductor model [4] to prove the capability to detect the parity of the system getting fundamental insight on the interplay of YSR and spin excitation, which are potential building blocks for topological superconductors and quantum computing.

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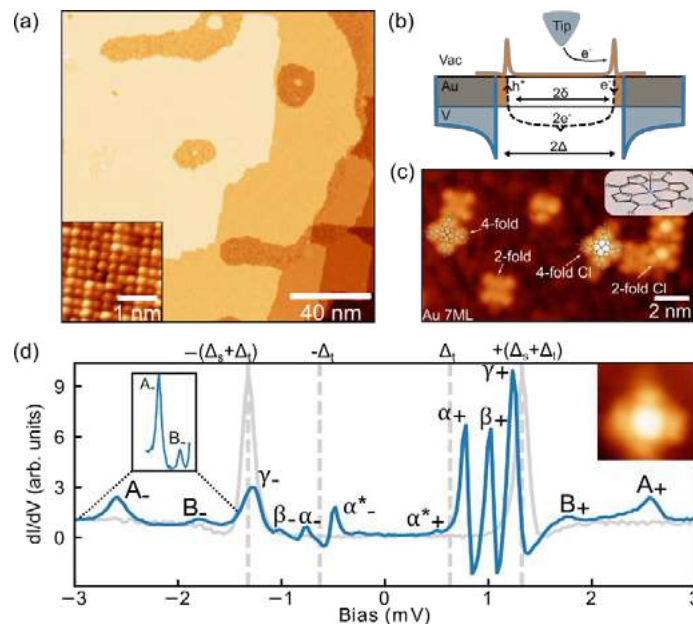


Figure 1: (a) Topographic image of the novel proximitized Au/V(100) system. Inset: atomic resolution of Au film. (b) Cartoon of the setup: electrons from the STM tip tunnel through the proximitized Au surface, probing the Andreev bound states. (c) Topographic image of the evaporated FeTPP-Cl molecules. Four different species are indicated. (d) Spectroscopic measurement of the 4-fold FeTPP-Cl molecule. Peak B is related to a pair-excitation, which enables the measurement of the local parity of the system.

Energy harvesting from Anomalous Nernst effect on Co/Pt multilayers

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The anomalous Nernst effect (ANE) is a thermomagnetic effect that can be exploited for energy harvesting to make use of wasted thermal energy from natural sources or from different electronic devices¹. The effect depends on the direction of the magnetization of the sample with respect to the direction of a thermal gradient. Thus, in order to maximize the ANE without applying any external field, it is very convenient to have the remanence of the system in a well-defined direction. Here we report on the ANE response of microscopic devices based on multilayers of Co/Pt with high perpendicular magnetic anisotropy². We fabricated micrometre sized devices to enhance the thermal gradient and achieve high efficiency thermoelectric devices. Consequently, the thermal decay occurs across a very small space, giving thermal gradients three orders of magnitude higher than the achieved in macroscopic devices. We extracted the magnetization of the microscopic structures from magnetic force microscopy (MFM) images. We also measured the maximum current and power provided by the device. We obtained record voltages of approximately 30 mV/cm and power densities of around 11 W/cm³. This work tries to emphasize the importance of evaluating the resistance or the maximum current admitted by materials with high ANE for energy harvesting purposes.

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Figures

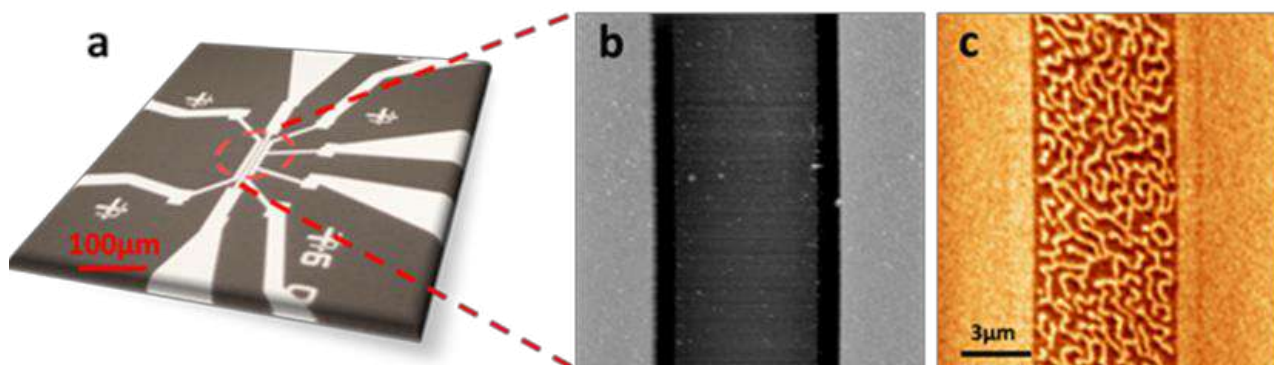


Figure 1: a) Picture of the device used to measure the ANE thermopower of microscopic multilayers. b) Atomic Force microscopy and c) MFM images of the magnetic multilayer without remanent magnetization, showing the worm-like structure of the magnetic domains.

Fabrication and characterization of exfoliated high-temperature superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ flakes for van der Waals heterostructures

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2D layered van der Waals materials are one of the most interesting and richest topics in condensed matter physics during the last decade due to their fascinating properties, including emergent phenomena which can arise from stacking materials with different properties [1]. $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO-2212) is one of the most studied high- T_c superconductors in which, depending on the hole doping, different quantum phases appear such as Mott insulator associated with an antiferromagnetic order, non-conventional superconductivity, strange metal or pseudo-gap phase [2].

In this work, we have characterized the properties of exfoliated BSCCO-2212 flakes with thickness between 20 nm and 100 nm, with the final aim of fabricating van der Waals heterostructures based on high- T_c superconductors. BSCCO-2212 loses its superconducting properties and becomes an insulator under environmental fabrication conditions [3]. In order to avoid the superconducting phase degradation different fabrication processes have been considered including optical lithography, electron beam lithography and viscoelastic stamping on pre-patterned electrodes in controlled N_2 atmosphere. Different optical characterization techniques were used to study the structural properties of the flakes, including optical contrast to study how the apparent color is related with the thickness of the material. By means of Raman spectroscopy, we have investigated how the superconducting phase degradation affects the structural properties of different thickness exfoliated flakes. Finally, by magneto-transport measurements as a function of temperature and in presence of high magnetic fields, their electrical properties have been studied, showing that, depending on the fabrication process and the exposure to ambient conditions, the flakes exhibit either superconducting or insulating behavior.

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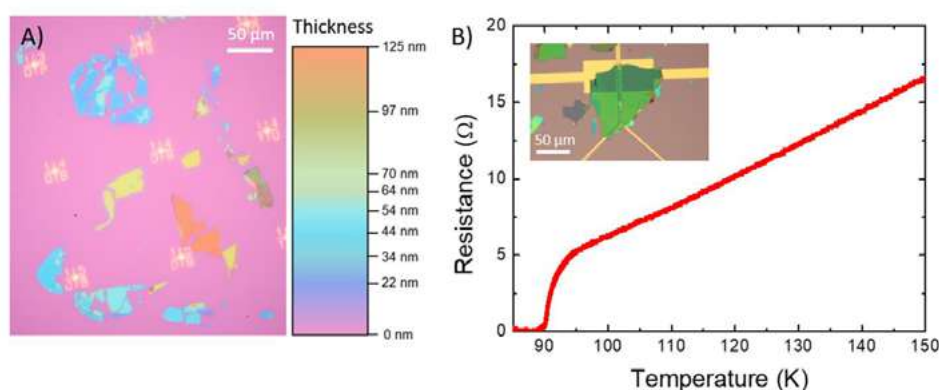


Figure 1: A) Exfoliated BSCCO-2212 flakes on SiO_2/Si substrate and scale bar relating color to thickness. B) Superconducting transition of a BSCCO-2212 flake exfoliated on top of pre-patterned electrodes.

Study of the Electrical Capacitance From Classical to the Quantum Regimen

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Using a Controlled Break Junction based on a Scanning Tunneling Microscope we can follow the evolution of the electrical capacitance as two electrodes are brought together. At large distances the capacitance increases following a classical behavior that can be described through the electrostatic analysis as derived from the geometrical characteristics of the electrodes. At shorter interelectrode distances a saturation of the capacitance, due to the consideration of the Quantum Capacitance of the system, is observed, followed by its exponential decrease from the tunneling leakage of charges through the junction. All the behavior above can be understood by Büttiker's theory for the capacitance in quantum systems [1-3].

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Figures

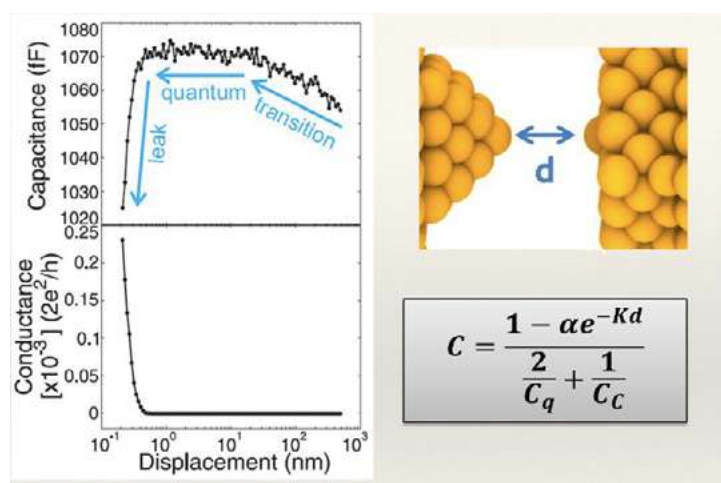


Figure 1: Evolution of capacitance with the interelectrode distance as understood by Büttiker's theory

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Development of hybrid Superconducting Single-Photon Detectors based on NbTiN and Graphene

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Superconducting nanowire single-photon detectors (SNSPDs) exhibit extremely high timing performance and sensitivity [1][2]. Nevertheless, their operating temperature is restricted to low temperatures ($T < 10$ K), increasing the cost and operation complexity [2]. In an SNSPD, a voltage pulse is obtained when a photon hits the nanowire, and it breaks Cooper pairs, generating a hotspot with a finite resistance. These detectors exhibit low dark count rate (DCR), low jitter, high detection efficiency, fast time response and polarization sensitivity. However, they have limitations related to the latching and reset dead time, and some frequency bands are not accessible due to constraints imposed by the superconducting bandgap [2]. Our objective is to manufacture hybrid systems based on conventional superconductors and graphene. Graphene would quickly release the thermal energy of the hotspot and lessen the latching effects due to its high thermal conductivity as well as expand the detection limit acting as an absorbent.

The NbTiN nanowires are produced via DC reactive magnetron sputtering with a thickness of 25 nm and optical or electron beam lithography onto SiO_x/Si substrate. Graphene is fabricated by chemical vapor deposition (CVD) and transferred on top of the nanowires. The characterization of the samples has been performed in a close-circuit cryostat setup (4 K). Preliminary results show a critical temperature (T_c) of 12.39 K in the NbTiN meanders without graphene. Both T_c and the critical current (I_c) show a shift towards lower values in the hybrid system which could be due to the superconducting proximity effect. In the IV curve of the hybrid system, we have observed an unstable region between the superconducting and non-superconducting state with a negative differential resistance, a significant reduction of the electrical hysteresis as well as several peaks. The dynamic response to pulsed light (488 nm) is up to 1 MHz and 800 kHz for meanders of the non-hybrid and hybrid systems, respectively. However, detection efficiency seems to be higher with graphene.

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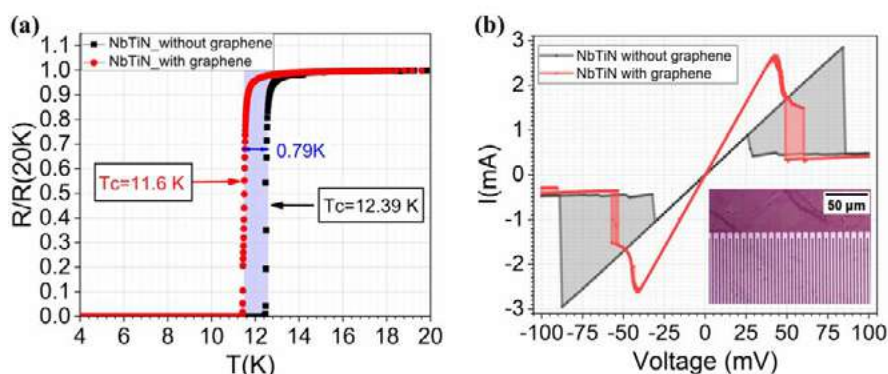


Figure 1: (a) Normalized RdT curves. (b) IV curves obtained at 3.8K of the NbTiN devices with and without graphene. Inset: Optical image of NbTiN meander with Graphene.

Engineering π -Magnetism in Carbon-Based Nanostructures

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Magnetic carbon-based materials and nanostructures have recently emerged as promising candidates for applications in spintronics and quantum computation, thanks to several appealing properties, such as long spin coherence times and long-range spin interactions [1].

While magnetism is missing among the properties of ideal graphene, an intrinsic spin polarization can develop in some graphene nanostructures with well-defined shapes, exhibiting an open-shell character, i.e., possessing one or more unpaired π -electrons. The high reactivity of these systems makes their growth and characterization particularly challenging. Recently, however, the advances of on-surface synthesis performed on metal substrates in ultra-high vacuum environments have allowed to fabricate open-shell carbon nanostructures with atomic precision and to investigate their electronic and magnetic properties by means of surface science techniques, such as scanning tunneling microscopy and spectroscopy.

Here we report our results on the characterization of magnetic interactions in spin-hosting carbon nanostructures on metal substrates. Firstly, we investigate the interaction between the two spin centers of an organic diradical, derivative of the Chichibabin's hydrocarbon, focusing on the influence of the molecular geometry on the spin coupling. Then, we present a more complex system, a triangulene-based hexamer, exhibiting fingerprints of collective spin excitations [2]. Our findings represent an important step towards the understanding and control of magnetic interactions within purely organic nanostructures.

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Electron paramagnetic resonance spectrometer based on lumped element superconducting resonators

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Electron paramagnetic resonance (EPR) spectroscopy is a widely used tool to detect and characterize paramagnetic species, such as some metal ions and organic radicals, with applications in various science fields such as physics, chemistry, material science and medicine. However, conventional EPR systems only allow studying macroscopic samples because the spins couple only very weakly to the microwave photons [1]. The detection and identification of certain proteins and molecules in samples of biological and environmental interest is then limited by the low spin concentration in these materials. New alternatives are being investigated for pushing the detection limit to its minimum.

Among them, using superconducting circuits as quantum sensors opens a new path for these developments. In fact, lumped element resonators (LERs), which consist of a series inductance-capacitance circuit [2], can act as very high efficient microwave cavities. Through a correct circuit design, the microwave photon that the cavity generates can be localized within a microscopic volume, thereby pushing the limits of sensitivity of the EPR spectroscopy by several orders of magnitude. Moreover, frequency multiplexing and tuneability of LERs allow characterizing spin transitions in the low magnetic field regime and the simultaneous characterization of different samples in a single chip.

As a proof of concept, we have developed an on-chip EPR device based on Nb superconducting LERs to sense the iron- and oxygen-binding protein metmyoglobin (Fe(III)-porphyrin) (from equine heart). We have checked the spectrometer sensitivity by depositing different amounts of these proteins on different LERs, going from microdroplets to a single molecular layer, deposited by means of dip pen nanolithography based on AFM. Low temperature spectroscopy measurements show that we can get weak coupling for all myoglobin protein samples. This sensitivity opens the path to the detection and characterization of micro-sized samples and even individual proteins. Further optimization of the LERs and pulsed measurements will be performed in order to develop a fully functional spectrometer for electron paramagnetic resonance characterization of microscopic samples.

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Bridging spin Qbits to superconducting circuits through carbon nanotubes

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Hybrid systems based on superconducting planar resonators strongly coupled to magnetic molecules are promising candidates for future large-scale quantum processors [1]. Superconducting microwave resonators allow the strong confinement of the electromagnetic fields mode volume, which is crucial for reaching a strong and coherent coupling with the spin qubits. However, achieving control over a few or single spins remains challenging. In this sense, two main issues need to be overcome. First, the cavity field effective volume needs to be further concentrated to maximize the addressability of a single spin in a controlled way. Second, as the microwave field is localized in a nanoscopic region, developing a method to deliver the magnetic sample with sufficient spatial accuracy is crucial. As a first approach, I. Gimeno *et al.* showed that reducing the width of a superconducting transmission line locally leads to an enhancement of the microwave magnetic field and, therefore, of the achieved coupling. Utilizing dip pen nanolithography, they can place nanodeposits in a controlled way, reducing the number of coupled spins by several orders of magnitude [2]. However, new approaches must be developed to achieve strong coupling to a single spin.

We propose to downscale and reach the single-spin sensitivity limit by replacing the constriction of the superconducting resonator with a carbon nanotube (CNT). This approach presents two significant advantages: first, it concentrates further the microwave magnetic volume, increasing the coupling rate to a single spin; second, as CNT can be directly functionalized with molecular species [3], it allows addressing a single magnetic molecule in a localized position. Preliminary results of a hybrid superconducting/CNT resonator are presented, where the controlled positioning of the carbon nanotube on the nanometer scale has been achieved by dielectrophoresis [4]. Moreover, optimized superconducting lumped element resonators (LERs) have been developed and coupled to CNT functionalized with magnetic porphyrin rings (mMINT) to estimate its feasibility as qubits measuring its collective coupling and decay rates.

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High cooperativity coupling to nuclear spins on a circuit quantum electrodynamics architecture

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Nuclear spins are candidates to encode qubits or qudits due to their isolation from magnetic noise and potentially long coherence times. However, their weak coupling to external stimuli makes them hard to integrate into circuit quantum electrodynamics architectures, the leading technology for solid-state quantum processors. Here, we study the coupling of $^{173}\text{Yb(III)}$ nuclear spin states in an $|\text{Yb(trens al)}|$ molecule to superconducting cavities. Experiments have been performed on magnetically diluted single crystals placed on the inductors of lumped-element LC superconducting resonators with characteristic frequencies spanning the range of nuclear and electronic spin transitions. We achieve¹ a high cooperative coupling to all electronic and most nuclear $|\text{Yb(trens al)}|$ spin transitions, a necessary ingredient for the implementation of qudit protocols with molecular spins using a hybrid architecture.

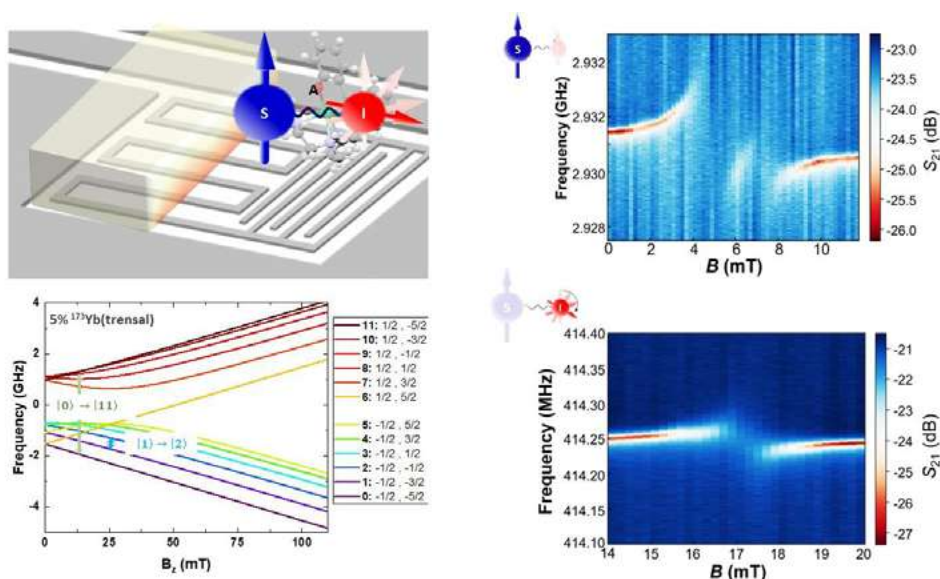


Figure 1: Left: Illustration of a single crystal of Yb-trens al molecules coupled to a lumped-element superconducting resonator (top) and scheme of electronuclear spin levels in $^{173}\text{Yb-trens al}$ (bottom). Right: 2D plots of microwave transmission experiments showing signatures of high cooperativity coupling of cavity photons to the 0-11 electronic spin transition (top) and to the 1-2 nuclear spin transition (bottom).

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EFFECT OF GALLIUM DOPING ON STRUCTURAL AND TRANSPORT PROPERTIES OF THE TOPOLOGICAL INSULATOR Bi_2Se_3 BY MOLECULAR BEAM EPITAXY

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Three-dimensional topological insulators (TIs) are described by massless Dirac surface states and reduced carrier scattering, due to the presence of strong spin-orbit coupling and the time-reversal symmetry (TRS). Bi_2Se_3 is one of the most promising TI due to its relatively large bandgap (0.3 eV[1]), which makes it the most suitable to work at room temperature. Recently, this material has been used to design materials exhibiting quantum anomalous Hall effect [1] and topological superconductivity [2], which are keys for the future of quantum computing. These topological properties can be achieved by doping with specific elements, such as Cu or Sr [2] however, studies with other elements are scarce. Here, we use molecular beam epitaxy (MBE) to grow high-quality single-crystal films of Copper and Gallium-doped Bi_2Se_3 . We report the effect of Ga doping with different concentrations on the structural, vibrational and electrical properties through XPS, Raman and XRD measurements, confirming the successful incorporation of the Ga [3] and Cu dopants. Through magneto transport measurements, we confirm that the n-type semiconductor character is maintained, while the bulk concentration is increased. Furthermore, a disappearance of the weak antilocalization effect (WAL) upon concentration suggest the suppression of the topological states.

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Figures

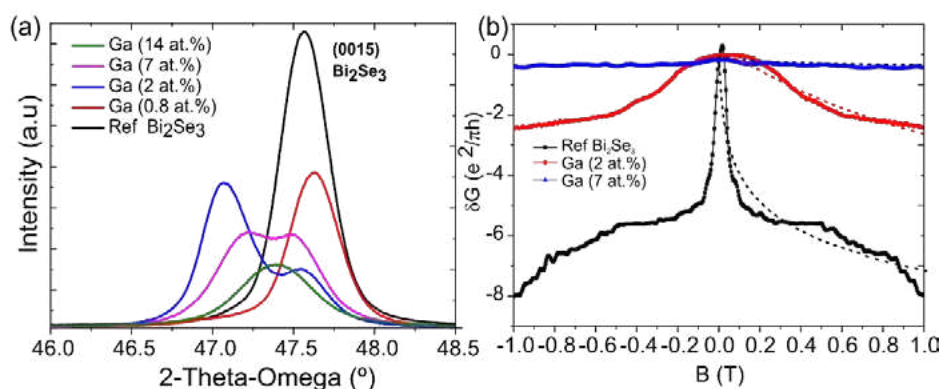


Figure 1: (a) XRD diffractogram for the Bi_2Se_3 doped with Ga and WAL measurements for undoped and doped Bi_2Se_3 as a function of low magnetic field with the corresponding fittings by the HLN model (dashed lines).

Spin-dependent polaron transport in helical molecules

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We study thermal effects on spin-transport along a deformable helical molecule in the presence of chiral-induced spin-orbit coupling [1]. The carrier-lattice interaction is modeled by the well-established Peyrard-Bishop-Holstein model [2] within the Langevin approach to include temperature as a stochastic noise. The carrier-lattice interaction causes the occurrence of polaron states in the molecule. We demonstrate the existence of two well-differentiated spin-dependent polaron transport regimes as a function of temperature. In the low-temperature regime, the spatial separation of the two spin-dependent polaron wave-packets results in a nonzero spin current. On the contrary, the spin current becomes negligible if the temperature of the system is high enough. Finally, we characterize this transition and estimate the critical temperature at which it takes place. Our results become relevant within the frame of the so-called chiral-induced spin selectivity (CISS), a new intriguing phenomenon that has attracted a lot of attention regard helical and other chiral organic molecules [3].

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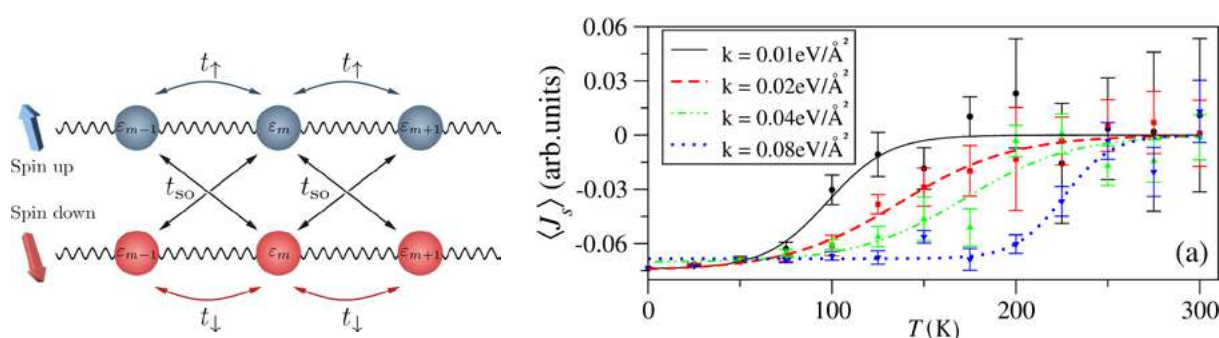


Figure 1: Left panel: Planar sketch of a deformable helical molecule. The parameters of the tight-binding Hamiltonian and the carrier and the spin-orbit (SO) coupling between neighboring sites are shown. Right panel: thermalized spin current for different values of the stacking potential parameter k as a function of temperature T .

Novel engineered architectures and phenomena in all-oxide freestanding interfaces

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Complex correlated oxides are quantum materials hosting a wide range of electronic groundstates with different functional properties controllable by external stimuli (magnetic/electric fields, light, strain etc). Doping level and strain states are sensitive knobs to tune the structure and composition of the oxygen sublattice which is strongly coupled to the electronic structure via crystal field splitting and valence band filling.

Epitaxial (cube on cube) growth on single crystalline substrates imposes stringent restrictions to the strain configurations experimentally available. The recent success in releasing epitaxial oxides from the substrate has opened exciting opportunities to tailor strain beyond the limitations of the epitaxial process [1-2]. Yet, the final strain map -and its functional properties at the nanoscale- is determined by the presence of uncontrollable defects generated mainly during the growth process.

Here we show a versatile technique to generate non-trivial strain patterns through the assembly of freestanding oxide layers. We will show that heterostructures combining ferroelectric freestanding BaTiO₃ thin films feature periodic strain configurations that can be manipulated *ad hoc* during the assembly process. The manifold of completely new strain configurations is expected to yield profound changes in ground-state properties and responses of the correlated oxides.

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Electronic properties of topological rough nanowires for thermoelectrical performance

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We study the electronic states in topological nanowires of narrow-gap semiconductors, such as PbTe or SnTe, with rough surfaces, using a continuous two-band model. We calculate the subband structure and identify topological conducting states located at the surface of the nanowire. In addition, a novel approach to study a nanowire with rough surface demonstrates that the topological surface states are mostly confined in the widest areas of the nanowire. This effect leads to a flattening of the subbands, thus raising the effective mass of carriers. Finally, we analyze the thermoelectric properties of the topological nanowires [1]. The reduction of the radius causes a noticeable enhancement of the thermoelectric efficiency due surface phonon scattering, as expected. However, we also observe that the appearance of topological surface states can play a detrimental role, reducing the thermoelectric efficiency. We conclude that, in addition to nanostructuring, the modulation of the radius of the nanowires, which partially suppress the conduction of the surface states, may be a potential strategy to improve the thermoelectric response of narrow-gap semiconductor nanowires.

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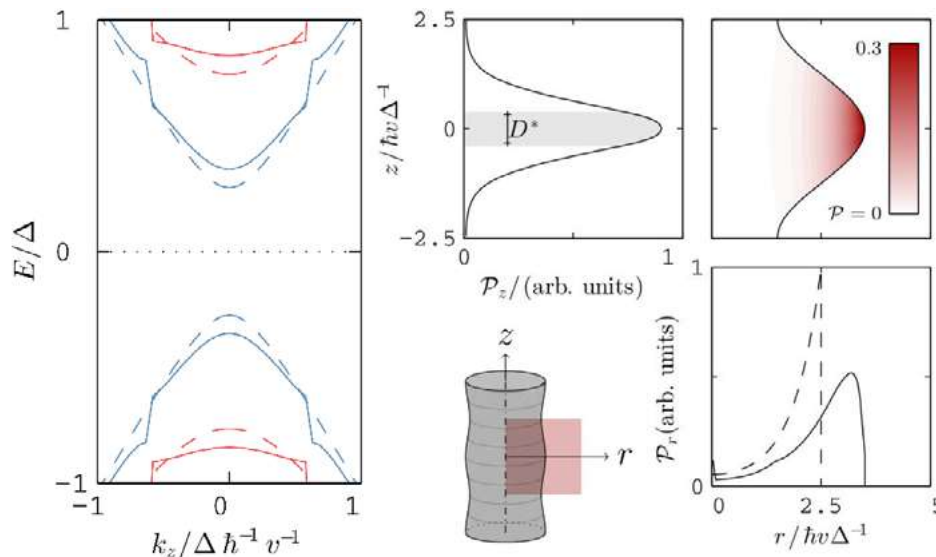


Figure 1: Energy spectra and probability density of a surface state in a rough nanowire of radii $R = 2.5 \hbar v / \Delta$, roughness amplitude $\delta R = \hbar v / \Delta$ and roughness period $D = 5 \hbar v / \Delta$. Subbands flatten when compared to a uniform nanowire, whose energy spectra is presented with dashed lines. Spatial probability density of a surface state is displayed. Its projection across the radial direction shows its localization next to the surface of the nanowire, as it also happens for a uniform nanowire, whose probability is displayed with dashed lines. Projection across the axial direction proves that surface states are mostly confined in the widest areas of the nanowire.

FABRICATION OF A NANOSQUID FOR THE STUDY OF QUANTUM MAGNONICS

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Quantum magnonics concerns the study of magnons, collective spin dynamics which propagate in magnetic materials as spin-waves or resonant modes, and takes them to the quantum limit of single-magnon excitations. Exploring their interaction with photons offers new possibilities to integrate them in quantum information systems, such as radiofrequency to optical signal transducers, microwave circulators, etc. With this aim, we must develop and study nanometric magnetic structures able to sustain localized excitations and to be coupled to photonic cavities or other quantum systems. The characterization of these structures [1] entails many complications: small and highly-localized magnetic moments need to be very well coupled to the sensor; magnonic modes in nanostructures are typically in the microwave range, so we need high time resolution and electronics suitable for high frequencies; systems must be studied at cryogenic temperatures around 10 mK, where thermal energy approaches the energy of magnonic excitations; finally, strong magnetic fields must be applied to tune the resonance frequency of the different magnetostatic modes or to induce the nucleation/annihilation of magnetic textures.

To meet all these conditions, we must use integrated superconducting circuits, able to operate in the radiofrequency regime without resistive losses, such as the SQUID (Superconducting Quantum Interference Device). Being among the most sensitive magnetometers to date, nanoSQUIDs may be scaled down to meet the coupling conditions and enhance sensitivity, being able to detect the magnetic moment of individual nanoparticles. SQUIDs are typically only used in dc measurements, due to the highly specific amplification techniques they require, which limit their frequency scope. Nonetheless, the Josephson effect persists up to radiofrequencies, making the nanoSQUID suitable to measure magnetization dynamics associated to magnonic excitations when incorporated in the right setup.

In this work we report on the fabrication and characterization of a nanoSQUID based on bicrystal grain boundary Josephson junctions in an epitaxially grown YBa₂Cu₃O₇/MgO thin film [2,3] which show, at low temperatures, high sensitivity, small inductance, low white noise, high critical current density and high in-plane critical field incorporated into a transmission line structure. This configuration will allow us to measure, with the same device: (i) hysteresis cycles – DC measurements –, (ii) relaxation and inversion dynamics – RF measurements – and (iii) ferromagnetic resonance. We use electronics and connectors suitable for RF and consider impedance matching in the superconducting circuit design in order to maximize the power transfer along the whole system.

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Traces of Majorana zero modes in spin-polarized persistent currents.

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The quest for Majorana zero modes in the laboratory is an active field of research in condensed matter physics. In this regard, there have been many theoretical proposals to detect them. However, their experimental detection remains elusive. Here, we present a realistic setting by considering a quantum ring with strong Rashba spin-orbit coupling and threaded by a magnetic flux, in contact with a topological superconducting nanowire. We focus on spin-polarized persistent currents to assess the existence of Majorana zero modes. We also find that the Rashba spin-orbit coupling allows for tuning the position of the zero energy crossings in the flux parameter space and has sizable effects on spin-polarized persistent currents. We believe that our results might contribute towards probing the existence of Majorana zero modes.

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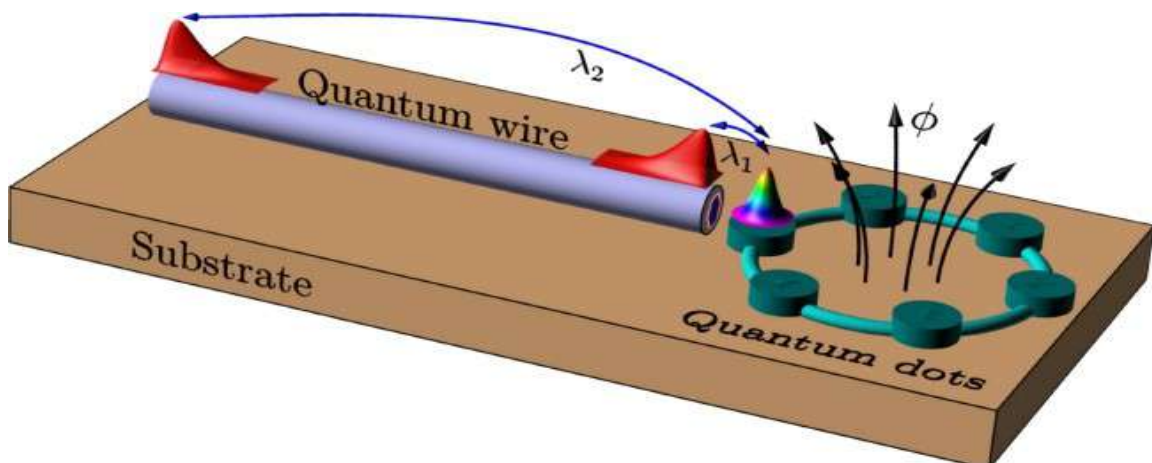


Figure 1: Schematic representation of the system under study. A nanowire driven into a superconducting regime supports a Majorana zero mode at each edge and influences the persistent currents of a quantum ring, threaded by a magnetic flux.

Structural spillage: an efficient method to screen amorphous topological materials

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While topological phases of matter are not restricted to crystals, there is no efficient method for predicting which amorphous solids are topological. In order to enable a high-throughput screening of amorphous topological materials, it is desirable to find a computationally efficient quantity, compatible with first-principle calculations. In this work, we introduce the structural spillage, a quantity that predicts the topological state of an unknown amorphous state by comparing it to a known reference crystal. To illustrate its potential, we benchmark it using tight-binding and first-principles calculations on two-dimensional amorphous Bismuth and its bilayer, showing a transition between $\mathbb{Z}_2 = 0$ and $\mathbb{Z}_2 = 1$ phases. Our work sets the basis to predict topological amorphous solids efficiently, opening up a large material class where to explore topological phenomena.

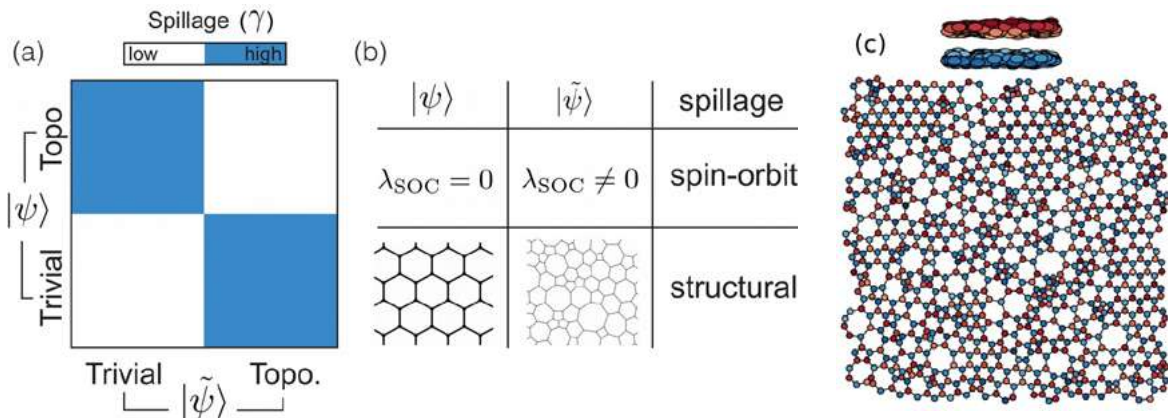


Figure 1:

(a) The spillage is high or low depending on whether a test wavefunction $|\psi\rangle$ is in the same or different topological state compared to a known reference wavefunction $|\tilde{\psi}\rangle$.

(b) The spin-orbit spillage (Liu and Vanderbilt, PRB 2014) compares two crystalline wavefunctions with and without spin-orbit coupling. The structural spillage introduced in this work takes advantage of the knowledge of the topology of a crystal to find whether an amorphous solid is in a trivial or topological state.

(c) Example amorphous structure used for the Bismuth (111) bilayer model.

Josephson junctions and nanoSQUIDs grown by Focused Ion Beam Induced Deposition (FIBID)

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Focused Ion Beam Induced Deposition (FIBID) is a direct-write resist-free nanolithography technique that enables the growth of high-resolution nano- and micro-structures. FIBID relies on a gas precursor that is injected into the area of interest and decomposed by a focused ion beam. Several precursors have been reported to produce superconducting deposits, as recently reviewed by us [1], among which $W(CO)_6$ is the most popular one. Using $W(CO)_6$, superconducting in-plane nanowires with 20 nm lateral resolution have been achieved [2], as well as three-dimensional superconducting helical nanowires [3]. In this contribution, we will present recent results on the fabrication of Josephson junctions and nanoSQUIDs based on FIBID-grown W-C deposits. First, results of W-C nanoSQUIDs patterned as two large pads connected by two short nanowires will be shown (Figure 1). In these devices, the critical current oscillates as a function of the externally-applied magnetic field, which results in a large output voltage to magnetic flux change (1.3 mV per magnetic flux quantum) [4]. Interestingly, these nanoSQUIDs can be implemented on a cantilever, which would find applications in scanning-SQUID technology. Secondly, experiments on Josephson Junctions (JJs) and nanoSQUIDs based on Bi_2Se_3 microcrystals and W-C superconducting contacts will be discussed. The obtained results indicate the coexistence of various oscillatory responses corresponding to the individual behaviour of the JJs and to the SQUID interferences [5].

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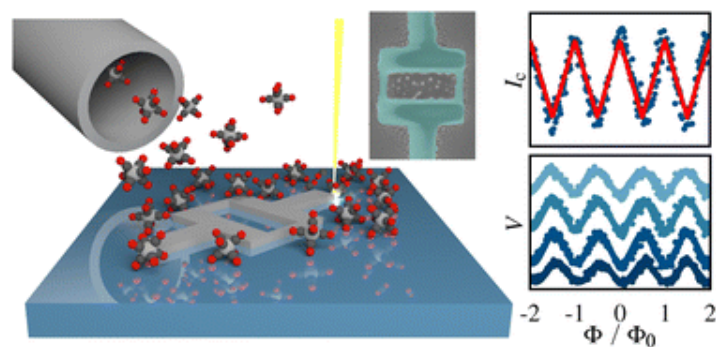


Figure 1: Sketch of the growth of a nanoSQUID based on W-C by FIBID, the resulting device and its response.

On the capacitive coupling of persistent current qubits

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Persistent current qubits are usually coupled to other elements via magnetic interactions. However, those interactions alone are only able to reproduce a small family of interacting models. In order to enlarge this family, we have analysed the capacitive coupling between persistent current devices. First, we present a general theory to find the effective interaction in the computational subspace, which works even in the ultra-strong coupling regime [1]. Then, we investigate three superconducting circuits designs that, thanks to the capacitive coupling, can emulate relevant low-energy Physics. The first one is a persistent-current qubit coupled to an LC resonator, see Fig1 (a). We have found that, by adding standard magnetic coupling, this system can simulate unexplored regimes of light-matter interactions. The second design corresponds to two flux qubits joined via a capacitor, see Fig (2) pannel (c). By adding magnetic interactions again, it displays an ultrastrong non-stoquastic low-energy Hamiltonian. In the last case, we explore a fluxonium qutrit capacitively coupled to a waveguide, which contains a quasi bound-state in the continuum with extremely long decaying times [2].

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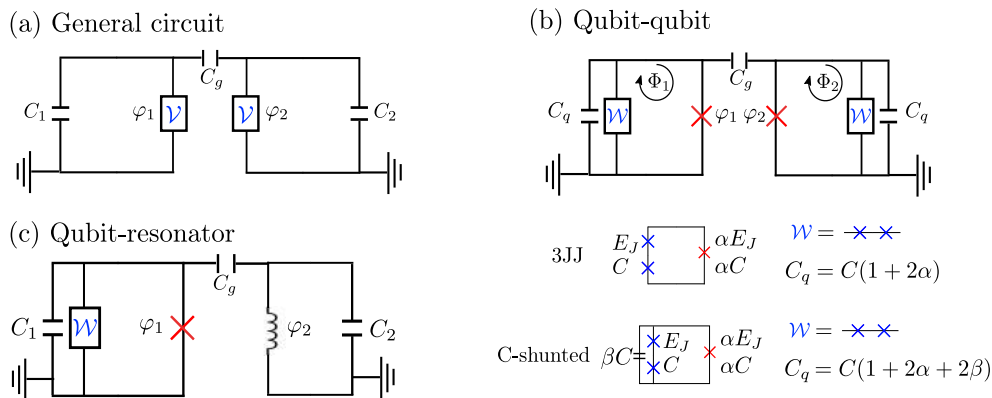


Figure 1: General coupling of two superconducting loops (a) Circuit diagram for two superconducting qubits coupled via a capacitor. (c) Circuit for a qubit and a resonator capacitively coupled. The elements denoted by W in the circuits (b) and (c) are for two Josephson junctions for the 3-Josephson junctions qubits.

Development of replicable SQUIDS from the control of the fabrication of Nb-based dayem bridge junctions

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Josephson junctions are the main constituents of superconducting quantum interference devices (SQUIDs), which combine the physical phenomena of flux quantization and Josephson tunneling. Due to their quantum behavior, they are fundamental elements in the development of quantum sensing and solid-state quantum computer.

SQUIDs have the ability to perform ultrasensitive magnetic flux measurements at low temperatures and in a broad frequency bandwidth. Therefore, they are commonly found in instruments such as amplifiers, magnetometers or gradiometers used in quantum sensing applications [1]. As for quantum computing, their variable inductance makes them suitable devices to act as tunable couplers, allowing to control the coupling between several elements, such as qubit-qubit interactions or qubit-quantum bus interactions [2].

One of the main challenges in the design and reproducibility of such systems, is the strong control needed over the fabrication process of the SQUID. To that end, in this work we propose the fabrication of Nb-based nanobridge Josephson Junctions. The target area is protected by a Pt layer grown by focused-electron-beam-induced-deposition (FEBID) and Focused Ion Beam (FIB) patterning is done with I₂ gas enhancing the etching rate and reducing the redeposited Nb. Higher control is achieved in the fabrication process attaining a better reproducibility rate.

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Figures

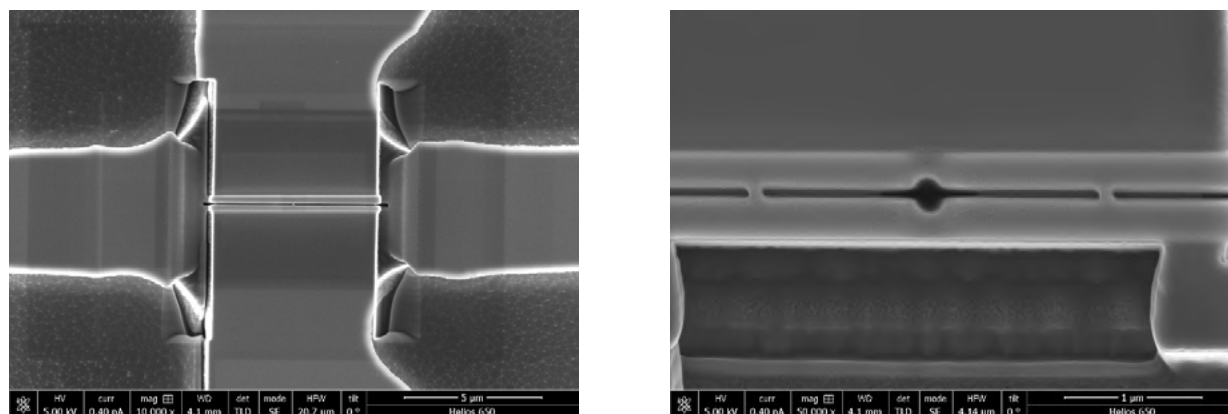


Figure 1: Caption of a nanobridge Junction (left) and a SQUID (right) with Pt deposited.

Suppression of the CDW and SC orders and emergence of short-range magnetic order in 6R-NbSeTe

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Abstract: 2D materials become a hot topic in recent years due to its promising physical, electrical, chemical, and optical properties. Here we show that upon 50% chemical substitution of Te for Se, superconductivity and electronic ordering in the 2D 6R-NbSeTe are strongly suppressed. Our combined structural data, high energy and VUV ARPES and DFT calculations support the 6R structural phase, with a dominant d_{z^2} and $d_{xy+x^2-y^2}$ character of the Nb bands at the Fermi level, which are barely affected by the Se-Te disorder. Magnetization measurements show a field dependent transition at ~60 K, without any anomaly in either resistivity or specific heat, pointing to a disorder induced short-range magnetic transition. These results highlight the effect of disorder to obliterate collective ground states in 2D materials and induced new quantum states of matter [1,2].

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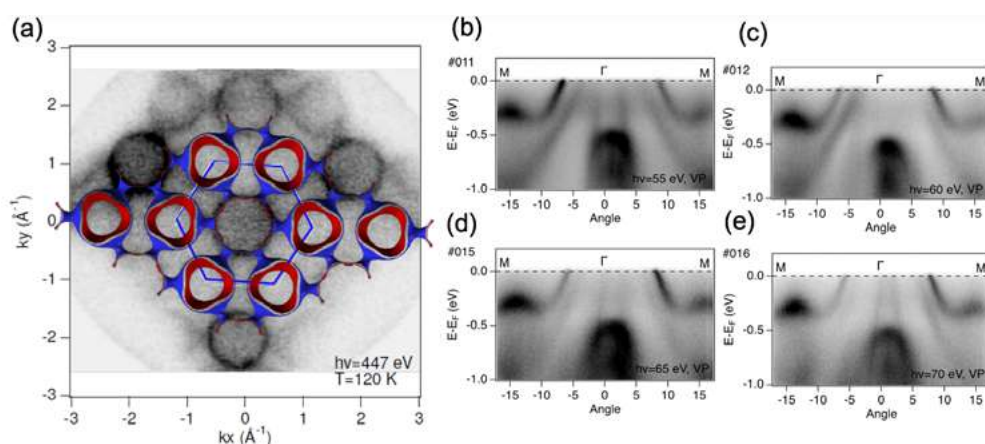


Figure 1: ARPES data of the 6R-NbSeTe crystals.

Study of defects under irradiated Fe through *ab-initio* techniques: cementite – Fe bcc interfaces

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The International Fusion Materials Irradiation Facility DEMO Oriented Neutron Source (IFMIF-DONES) Project is one of the three pillars on which the Fusion Program is founded. Its main goal is to study the irradiation damage that different materials will experience within fusion reactors. A 40 MeV, 125 mA deuteron accelerator will create a 14 MeV neutron flux of $10^{18} \text{ m}^{-2}\text{s}^{-1}$, which can produce displacement cascades and transmutation products, thus changing the macroscopical properties of the materials used to build the reactor. It is well-known that C impurities strongly affect defect evolution in Fe-based alloys [1]. Our goal hence is to determine where does C tend to locate in bcc Fe lattices: grain boundaries, loops, cementite... To understand this, DFT is used to determine formation, migration and binding energies of several point defects and structures.

A Fe bcc - cementite – a Fe and C compound found in all steels – interface is constructed in order to understand how defects behave in such grain boundaries, and whether they act as defect attractors or, on the contrary, they migrate away from the interface.

Finally, the interface is characterized for paramagnetic cementite using Constrained DFT for noncollinear magnetism [2].

All these properties are studied using DFT as implemented in the Vienna Ab Initio Simulation Package (VASP) [3]. Projector-Augmented-Wave (PAW) Pseudopotentials are used to describe electron-core interactions. Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional is used [4] within the generalized gradient approximation (GGA).

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Simulations of a micro positioner and PCB design for measurement of SQUIDs

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In this work, we present the design and fabrication of a micro positioner [1] based on two complementary approaches. The first one employs capacitive actuators to implement movement in the x-y plane [2]. On the other hand, C-MOS compatible piezoelectric materials will be used to control the displacement along the z axis [3]. Here we present preliminary simulations performed with COMSOL Multiphysics that allow us to fine tune the geometrical parameters of the positioner considering different types of materials. In addition to that, simulations are used to estimate the resistance, Von Mises stress, shear forces, torsion forces and elastic constant which serve to calculate the final effective displacement and response of the device. The resulting micro positioners will be combined with ultrasensitive magnetic sensors such nanoSQUIDs (Superconducting QUantum Interference Devices) [4]. In this way, it will be possible to displace nanometric samples in close vicinity to the most sensitive regions of the nanoSQUID, to perform scanning magnetic imaging and reference measurements. In this poster, we present the progress made so far in this doctoral thesis work.

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The Interaction of a Levitating Sphere with Helium Superfluids

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We have developed an apparatus for fine control of the motion of a superconducting sphere. The sphere can levitate in the bulk of a superfluid and is promising to be suitable for a wide range of measurements in both superfluid ^4He and ^3He [1]. Our finite elements analysis shows that the sphere can be driven in oscillatory motion, which will make a connection with numerous previous experiments in superfluids. Most importantly, the sphere can be made to move at a uniform velocity in a circle as well as in a straight line. This opens a whole new multitude of approaches to quantitative studies of superfluid quantum matter, including the study of heat radiation and transfer for objects detached from the wall immersed in superfluid at ultra-low temperatures. We will study both theoretically and experimentally the heat emission and absorption of the sphere [2, 3] when placed in a ^4He bath due to the phonon's excitations.

Upload a single .pdf file with a maximum size of 10Mb

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Figures



Figure 1: Superconducting ball levitating in superfluid ^4He at 1.5 K.

Quantum dot Josephson junction in a hybrid superconductor-semiconductor transmon device: a novel route for Andreev spin qubits

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I will discuss the physics of a hybrid superconductor-semiconductor qubit device [1] in which the Josephson effect is controlled by a gate-defined quantum dot in an InAs/Al nanowire. Microwave spectroscopy in such transmon circuit allows to probe the ground state parity of the quantum dot Josephson junction as a function of gate voltages, external magnetic flux, and magnetic field [2]. The measured parity phase diagram is in very good agreement with that predicted by the superconducting single-impurity Anderson model. This allows to tune the hybrid superconductor-semiconductor transmon device to be in a spin-1/2 ground state with an unpaired quasiparticle. Interestingly, a finite spin-orbit coupling results in two flux-sensitive branches in the transmon spectrum, depending on the spin of the quasi-particle. Manipulation and control of a direct spin-flip transition using all-electrical control [3] enables the implementation of a novel Andreev spin qubit. Embedding the Andreev spin qubit in a superconducting transmon qubit, allows to demonstrate strong coherent qubit-qubit coupling [4].

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Spin Relaxation in corrugated Graphene

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Controlling spin relaxation rate is important to design devices intended to be applied in spintronics. Since spin injection and detection was demonstrated, graphene has been considered to be applied for spintronic devices. One reason is its low spin-orbit coupling, that allows spin to travel further while can be modified via proximity effect with other materials (such as TMDs). However, studies report spin relaxation times orders of magnitude lower than predicted by theory. This could be due to the appearance of “local” spin orbit coupling due to ripples as reported by Guinea et al. [2]. Here we develop a KPM (Kernel Polynomial Method) real space approach [1] study to estimate the contribution of corrugation to the spin dynamics of a corrugated graphene sample in a wide range of gate voltages and make a discussion based on the main spin relaxation processes known.

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Figures

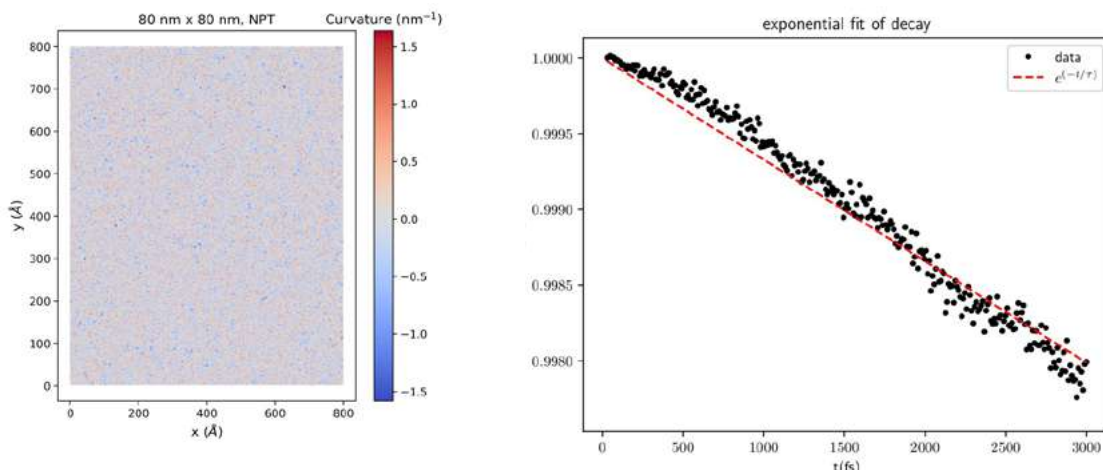


Figure 1: Spin relaxation time for a corrugated graphene sample and characterization of the sample. Left figure curvature profile where blue is for negative curvature and red for positive curvature and right figure is a spin relaxation graph fitted with an exponential decay used to obtain relaxation time

The singular manifold method and soliton-like solutions for Nonlinear Schrödinger Equation

Presenting Author P. G. Estévez

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We study an effective integrable nonlinear model describing an electron moving along the axis of a deformable helical molecule. The helical conformation of dipoles in the molecular backbone induces an unconventional Rashba-like interaction that couples the electron spin with its linear momentum. In addition, a focusing nonlinearity arises from the electron-lattice interaction, enabling the formation of a variety of stable solitons such as bright solitons, breathers, and rogue waves. A thorough study of the soliton solutions for both focusing and defocusing nonlinear interaction is presented and discussed

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Figure I

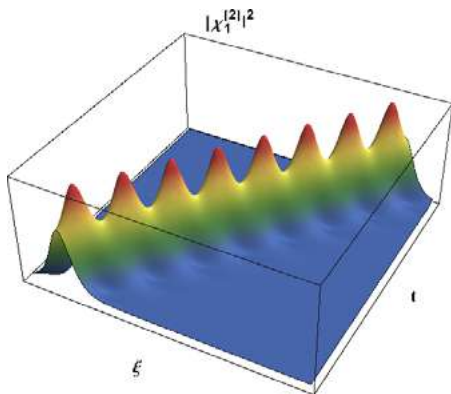


Figure 1: Generalization of the Kuznetsov-Ma breather

Figure II

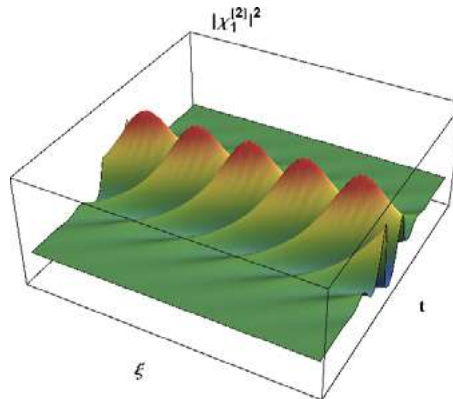


Figure 1: Generalization of the Akhmediev breather

Hot electron dynamics in graphene – a linear-scaling atomistic approach

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Graphene holds significant promise for a variety of applications. In particular, graphene photodetectors have been shown to be very fast, highly sensitive, and consume minimal power, making them extremely promising for next-generation optical communication technologies [1].

Hot electrons – electrons whose temperature is higher than the surrounding lattice – play a fundamental role in such graphene photodetectors. A variety of theories and measurements have been developed and conducted to understand the main factors controlling the dynamics and relaxation of hot carriers in graphene, but fundamental questions remain to be examined [2].

In this talk, we present our development of a numerical simulation tool that can capture the dynamics of hot carriers in graphene with arbitrary lattice vibrations, defects, and disorder. Our methods are linear-scaling, meaning we can simulate systems with millions of atoms – this permits an atomic description of the system while allowing for system sizes that approach the experimental scale. Such a tool will allow for a deeper fundamental understanding of hot carrier dynamics in graphene, as well as reveal strategies for the control of such dynamics, with an eye toward future applications in photodetection, optical communications, and energy conversion.

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Figures

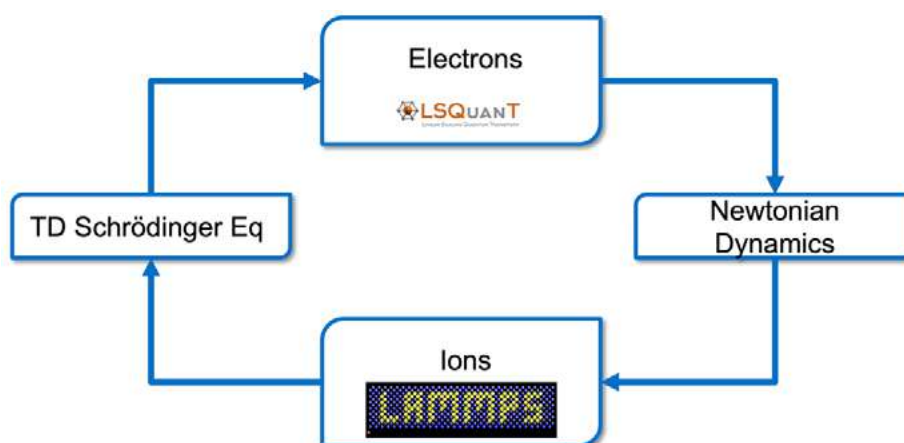


Figure 1: schematic representation of the self-consistency cycle for the atomistic simulation of coupled charge and ion dynamics

Metal-Protein-Metal Junctions: Electron Transport and Mechanical Deformation

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Proteins have proven to be promising candidates for molecular electronics, showing in some cases much higher conductance than one would naively expect from their size. In particular, the blue-copper azurin extracted from *Pseudomonas aeruginosa* has been the subject of many experimental studies, although the exact transport mechanism is still under debate. Here I will present our efforts towards understanding the origin of such interesting effects from a theoretical perspective, analyzing both the electronic structure and the geometrical arrangement [1-6].

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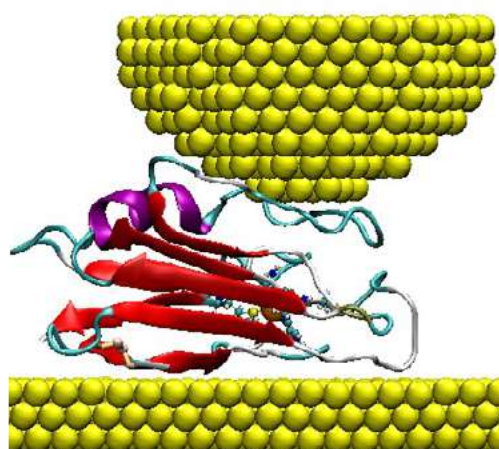


Figure 1: Gold-protein-gold junction based on the blue-copper azurin from *Pseudomonas Aeruginosa*.

Magnetically-diluted two-dimensional Co^{II}Rh^{III} bimetallic oxalates as quantum spin liquid candidates

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A quantum spin liquid (QSL)[1] is an elusive state of spin matter characterized by the absence of long-range magnetic order, even at zero temperature, and by the presence of exotic quasiparticle excitations. In spite of their relevance for quantum communication, topological quantum computation and the understanding of strongly correlated systems, like high-temperature superconductors, the unequivocal experimental identification of materials behaving as QSLs remains challenging. Here, we present a novel 2D heterometallic magnetically-diluted oxalate complex meeting all key requirements to become a QSL: a low spin ground state, determined by spin-orbit coupling, a magnetically-frustrated triangular lattice due to the presence of antiferromagnetic correlations, strongly suppressed direct exchange interactions and the presence of equivalent interfering superexchange paths between Co centres. A combination of specific heat and ac magnetic susceptibility measurements in a wide range of frequencies and temperatures show the presence of strong antiferromagnetic correlations concomitant with no signs of magnetic ordering down to 15 milliKelvin. These results show that magnetically diluted oxalates are therefore appealing QSL candidates as well as versatile systems to chemically fine tune key aspects of a QSL, like magnetic frustration and superexchange paths geometries.

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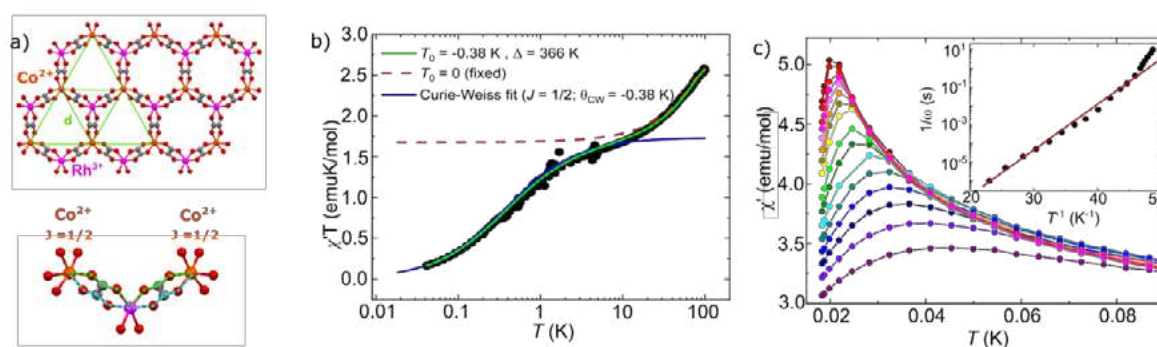


Figure 1: (a) In-plane structure of the oxalate-based bimetallic layer. $\chi'T$ as a function of temperature. The two drops in $\chi'T$ can be reproduced by a model that includes an excited spin doublet and spin-spin antiferromagnetic interactions between neighbours (green curve). (c) χ' measured from 15.85 mHz (dark red) to 158 kHz (dark purple) and down to $T = 15$ mK. No magnetic order is observed down to the lowest temperatures.

Towards hybrid van der Waals Josephson junctions based on NbSe₂

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The emergence of van der Waals heterostructures has paved the way for a “designer” approach, in which novel devices and new physics can be obtained by combining the properties of different two-dimensional materials. Among the many possibilities in this context, heterostructures based on superconducting few-layer NbSe₂ attract great interest for studying Josephson effects and the superconducting proximity effect in 2D systems [1]. Interestingly, recent work has reported on signatures of a topological superconducting phase in heterostructures based on NbSe₂ and 2D ferromagnets [2]. Moreover, first demonstrations of magnetic vdW Josephson junctions have been recently reported using a similar material combination [3]–[6].

Motivated by the above developments, we present here our first steps towards the fabrication of heterostructures based on NbSe₂, including our first attempts to fabricate Josephson junctions. In particular, we explore different ways to minimize residues and disorder in our samples which, we believe, is the culprit for not observing a conventional Fraunhofer interference pattern. We also report on our preliminary developments towards the fabrication of Josephson junctions with magnetic tunnel barriers.

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Electronic transport experiments and topography images in Tellurium

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Thanks to the nature of the tellurium and its hexagonal lattice, it is possible to find parallel helical structures, which usually are named as $P3_121$ and $P3_221$ chains. Recent studies in tellurium nanowires have demonstrated that the chirality of these helicoidal structures has a role in the charge-to-spin conversion[1].

In this work, we pretend to find and characterize these tellurium helicoidal chains via Scannelling Tunneling Break Junctions approach. However, as first steps, we have studied the electronic transport of tellurium nanocontacts at different conditions of temperature and pressure. Moreover we have used the STM topographic images in order to identify the facets that show these chiral chains.

The main objective of our research is to elucidate the existence of Te helicoidal chains $P3_121$ and $P3_221$ through the analysis of conductance versus the relative displacement of the electrodes.

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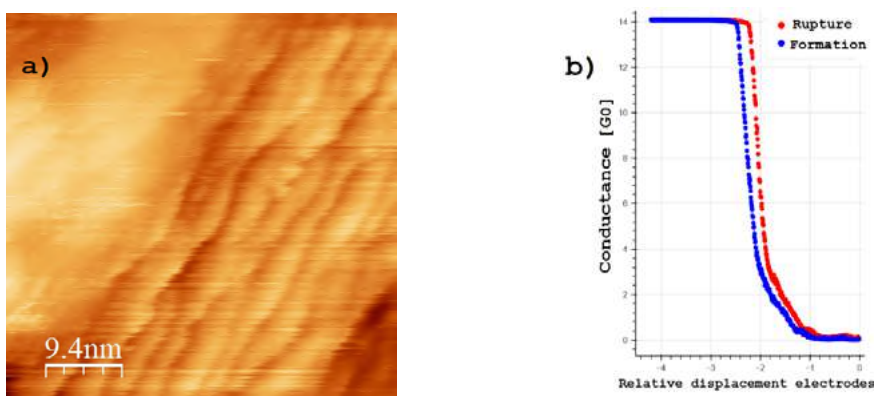


Figure 1: a) STM image of a Te 27×27 [nm] Bias 1.2 [V]. b) Conductance [Go] in function of Piezo Voltage in Te obtain in STM-BJ

Vortex lattice at high magnetic fields and charge density wave in $\text{KCaFe}_4\text{As}_4$ and $\text{CaK}(\text{Fe}_{0.988}\text{Mn}_{0.012})$

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The 1144 $\text{CaKFe}_4\text{As}_4$ compound is a pnictide superconducting material showing optimal superconducting critical temperature with T_c 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 T_c 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 $\text{CaKFe}_4\text{As}_4$ 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 $\text{CaKFe}_4\text{As}_4$. 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 $\text{CaKFe}_4\text{As}_4$ 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 $\sqrt{2}a_0 \times \sqrt{2}a_0$ where a_0 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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Superconductivity and band structure of AuSn₄

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The orthorhombic compound AuSn₄ is compositionally similar to the nodal line semimetal PtSn₄ [1], which stands out due to reports connecting topological properties of its band structure with its huge magnetoresistance [2,3]. Contrary to PtSn₄, AuSn₄ is superconducting below $T_c = 2.35$ K [4]. Recent work presents indications for two-dimensional superconductivity and for weak anti-localization [5] in magnetotransport in AuSn₄. Here we measure the superconducting density of states and band structure of AuSn₄ through Scanning Tunneling Microscopy (STM) and Angular Resolved Photoemission Spectroscopy (ARPES). We determine the shape of the superconducting density of states and the Fermi surface. We find several large circular electron pockets and a superconducting gap whose size ($\Delta = 0.46$ meV) is close to the one expected from BCS theory. The band structure calculated with Density Functional Theory (DFT) follows well the results of ARPES, except that DFT shows a much more pronounced anisotropy. Furthermore, we observe superconducting features in the tunneling conductance up to temperatures about 20% larger than bulk T_c . We discuss the crystal structure of AuSn₄ and show that, contrary to similar compounds as PtSn₄, there are two possible stacking of Sn layers, giving two nearly degenerate polytypes. The presence of polytypes in a strongly three-dimensional metal makes AuSn₄ a rather unique case where a variety of properties, mechanical and electronic, present features like those found in layered compounds.

More information at <https://arxiv.org/abs/2205.09975>.

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Tunneling spectroscopy through the magnetic phases of $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$

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CeRu_2Si_2 is an archetypical heavy fermion compound with a large electronic specific heat at low temperatures and no magnetic order. Application of a magnetic field produces a polarized phase through a metamagnetic transition at 8 T. CeRh_2Si_2 presents AFM order below about 36 K. $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$ shows a combined behavior, with an antiferromagnetic phase (AFM) below 5 K, which vanishes above 2.5 T, and a metamagnetic transition at 5.5 T. The electronic properties of $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$ are highly susceptible to a magnetic field, as shown by a strong magnetic field dependent specific heat and thermopower that changes sign with field. However, the magnetic field dependence of the electronic band structure is still unknown. Here we present atomically resolved tunneling spectroscopy studies in a millikelvin Scanning Tunneling Microscope across the magnetic phase diagram. We visualize directly atomic site dependent Kondo hybridization and show how the electronic band structure originates magnetic order.



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Magnetic field induced increased d-electron overlap in Au-Au junctions

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Although Au is the “noblest of all the metals”, it presents strong bonds and forms many alloys with other metals. The particularly large length of bonds between Au atoms reduces the overlap between d-states, favoring metallic connections and explaining effects as aurophilicity, the tendency towards aggregation of Au containing molecules. Au-Au atomic size junctions can be studied by measuring the conductance between two Au electrodes using a Scanning Tunneling Microscope (STM) and approaching both electrodes in a controlled way. Atomic size contacts form and present conductance quantization at $G_0 = h/2e^2$. Au-Au atomic size contacts form at particularly small conductance values, or equivalently at large Au-Au distances. Here we study Au-Au atomic size contacts under magnetic fields up to 20T. We show that the conductance for the formation of Au-Au junctions is increased by the magnetic field, evidencing a magnetic field induced reduction in the Au-Au distance. Furthermore, the conductance presents values smaller than the quantum of conductance $G_0 = h/2e^2$ at high magnetic fields. Our data show that there is an unexpected influence of a magnetic field on Au d-electron states. We discuss spin transport under a magnetic field in small d-electron systems, and possible consequences of the observed behavior.

Topological phase diagram of amorphous 2d $\text{Bi}_x\text{Sb}_{1-x}$ alloys from its entanglement spectrum

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In a previous work [1], we showed that it is possible to train a neural network with the entanglement spectrum of a solid, to distinguish between trivial and topological phases of a model, even in presence of high structural disorder and gap closings. On the other hand, $\text{Bi}_x\text{Sb}_{1-x}$ alloys are known to be topological insulators, both in 3d and 2d [2]. Then, we expect that as the alloy becomes amorphous, the alloy remains to be topological for some concentrations. We test this hypothesis computing the phase diagram for the 2d alloy as a function of disorder and concentration. For small disorder, the disorder itself produces the band inversion, effectively renormalizing the required spin-orbit coupling. We also characterize the alloys at strong disorder, where the material becomes gapless.

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Figures

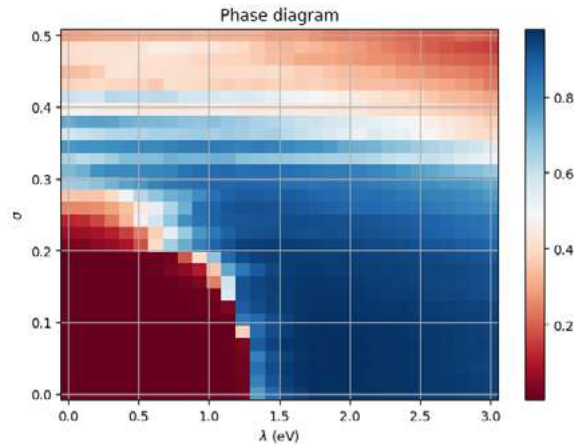


Figure 1: Topological phase diagram of 2d Bi as a function of disorder and spin-orbit coupling.

Joule heating effects in superconducting InAs nanowire islands

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Mesoscopic superconducting islands in hybrid superconductor-semiconductor nanowires have been intensively studied in the context of topological superconductivity, motivated by their potential for the realization of a topological qubit [1]. Interesting experimental results have been reported in the past years, including a 2e-to-1e transition in the periodicity of Coulomb oscillations and a related dependence with the island length, which has been interpreted in favor of topology and of exponential protection of Majorana zero modes [2-4]. Theoretical work has also put forward proposals for employing islands for realizing a topological quantum computer [1]. Heating effects, however, have not been considered in the interpretation of the above experiments, nor has its impact been evaluated in the context of proposals for quantum devices.

In this work, we study Joule heating in devices based on hybrid mesoscopic Al/InAs islands. To this end, we employ a technique that is able to detect the transition of superconducting parts of a hybrid device to the normal state [5]. Such transitions manifest as dips in the differential conductance, reflecting the suppression of Andreev excess current [6], and can be readily detected by employing typical DC measurement schemes. We use this signal as a tool to study the dissipation of heat generated by the Joule effect in mesoscopic islands. Interestingly, we show that the islands undergo a transition to the normal state at relatively low powers - ~ 100 pW. We evaluate the impact of Joule heating for typical device operation conditions.

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Spin-phonon coupling in antiferromagnetic Cr_2O_3 Nanocrystals

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A detailed Raman spectroscopy study of the lattice phonon modes and magnetic excitations in Cr_2O_3 nanocrystals with two different average sizes, in which the interplay between lattice dynamics and magnetism has been performed. Besides the spectral features characteristic of this antiferromagnetic material, small lattice distortions that precede magnetic ordering are also identified. Namely, we observe a general decrease of the phonon frequencies upon increasing the laser power (and therefore the local temperature) except for the $\text{E}_g(2)$ phonon mode, which shows an increase of its frequency and provides direct evidence of the coupling between the crystal lattice and spin configuration. We associate this spin-phonon coupling to a variation of the Cr-O-Cr angle/distance and, consequently, to a modulation of the local short-range magnetic order, which is observed to persist well above the onset of the Néel transition temperature.

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A group-theoretic approach to chirality-induced spin selectivity in molecular junctions

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Spin-orbit coupling gives rise to a range of spin-charge interconversion phenomena in non-magnetic systems where certain spatial symmetries are absent. Chirality-induced spin selectivity (CISS), a term that generically refers to a spin-dependent electron transfer in non-magnetic chiral systems, is one such case; appearing in a variety of seemingly unrelated situations ranging from inorganic materials to molecular devices. In particular, the origin of CISS in molecular junctions is a matter of an intense current debate [1,2]. Here we contend that CISS can be generally and fully understood on the basis of a symmetry analysis of the complete molecular junction, and not only of the molecule. Our approach, which draws on the use of point-group symmetries within the scattering formalism for transport, shows that electrode symmetries are as important as those of the molecule when it comes to the appearance of CISS. It turns out that standalone metallic nanocontacts can exhibit spin-polarization when relative rotations which reduce the symmetry are introduced. As a corollary, molecular junctions with achiral molecules can also exhibit spin polarization along the direction of transport, provided that the whole junction is chiral in some way. This formalism also allows to predict the qualitative changes on the spin-polarization upon substitution of a chiral molecule in the junction with its enantiomeric partner. Quantum transport calculations based on density-functional theory corroborate all of our predictions and provide further quantitative insight.

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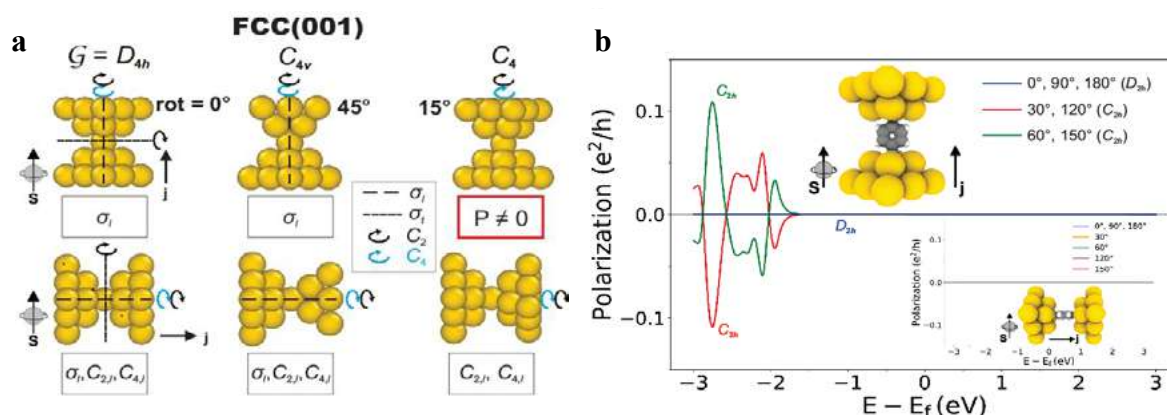


Figure 1a: The spin-polarization of the outgoing current is in principle a rather general feature, but due to the presence of certain spatial symmetries (indicated below each pair of contacts) it is forbidden in junctions with some specific point groups. **Figure 1b:** The qualitative role of the molecule is the reduction of the symmetry of the system, hence its anchoring is crucial to the induction of spin-polarization. The direction of this vector quantity is determined by the spatial symmetries of the junction.

Nanopatterning of hBN/WSe₂/hBN heterostructures for photonic applications

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The discovery of bright emission in two-dimensional (2D) monolayer transition metal dichalcogenides opened new avenues for the development of an ultracompact and flexible technological platform [1]. Moreover, it has been shown that their optical properties can be improved significantly by embedding them between high band-gap hexagonal boron nitride 2D crystals [2]. For many applications in photonics, it would be very interesting to pattern sandwiched hBN/WSe₂/hBN heterostructures with desired shapes while preserving their optical quality. It is particularly interesting the possibility of fabricating confined pillar-like structures where single photon emitters by quantum confinement or defect engineering could be fabricated.

In this work, we have fabricated pillar hBN/WSe₂/hBN structures with high optical quality as shown by micro-photoluminescence. Interestingly, our preliminary results show a similar intensity and emission energy in all the patterned pillars in contrast with the pristine sandwiched heterostructure that present variable strain-related emission energy shifts at different positions. Our results might open interesting possibilities for the fabrication of nanostructures based on 2D optical active materials, including site-controlled quantum emitters [3].

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Plasmonic Rectification of terahertz radiation using encapsulated graphene field effect transistor

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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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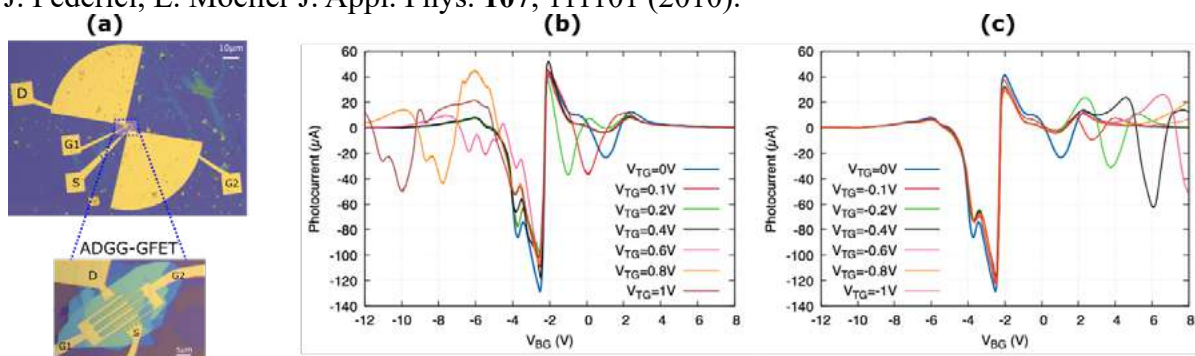


Figure 1: (a) Microscope photo of the ADGG-GFET and the measured photocurrent versus the back gate under excitation of 288GHz and at 1.7K for (b) positive top gates biases and (b) negative top gate bias

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Directional Light Amplification in Perovskite LEDs by Hybrid Photonic-Plasmonic Modes

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Halide perovskites show excellent optoelectronic properties including bandgap tunability, high radiative recombination rates and narrow emission lines that make them promising candidates for the next generation LEDs.^{1,2} However, their thin film character is yet to be exploited to enable full control over the emission properties, opening avenues to surpass the luminous efficacies of conventional LEDs and facilitating their widespread adoption.³

In this talk, we present a novel green perovskite LED architecture where enhanced emission and directionality on demand are achieved by means of a hybrid photonic-plasmonic structure. We show how a code based on the transfer matrix model boosted by a genetic algorithm identifies the best combination of materials and thin film thicknesses to maximise outcoupled light with very narrow and controllable angular dispersion, all in a realistic fashion compatible with the fabrication of efficient LEDs. This strategy leads to hybrid photonic-plasmonic modes highly confined throughout the whole cross-section of the perovskite emitter while ensuring a good band alignment of the building blocks for efficient charge carrier injection and radiative recombination.

The experimental realisation of the optimum designs allows us to demonstrate devices with amplified green emission selectively enhanced at different angles. Our low temperature process can tune the perovskite thickness on a nanometric scale to enhance electroluminescence on demand from the forward direction (0°) to up to 40°. This approach expands the role of the perovskite film from a mere emitter to an active photonic layer participating in the strong interference phenomena arising from the designed photonic-plasmonic nanostructures. This strategy is truly unique as opposed to standard methods where emitters are just embedded into the optical cavities. Our methodology is versatile and easily integrable into cost-effective perovskite LEDs with emission lines covering the entire visible spectrum. Thereby opening avenues for their application in displays and light sources where control over angular dispersion of light is crucial.

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